10/749,450

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1129pxo

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 11	CA/CAplus enhanced with more pre-1907 records
NEWS 7	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 8	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 13	OCT 19	E-mail format enhanced
NEWS 14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 18	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 19	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 20	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 21	NOV 13	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 22	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 23	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 24	NOV 20	CA/CAplus patent kind codes will be updated
NEWS 25	DEC 01	CAS REGISTRY updated with new ambiguity codes

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 04:28:36 ON 11 DEC 2006

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.78	3.78

FILE 'REGISTRY' ENTERED AT 04:39:37 ON 11 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4
DICTIONARY FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

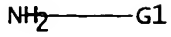
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10749450.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G2

G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G2 Ag,Cd,Co,Cu,Fe,Hg,Ni,Zn

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1
SAMPLE SEARCH INITIATED 04:40:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    34809 TO ITERATE

  5.7% PROCESSED     2000 ITERATIONS                                  2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       685030 TO   707330
PROJECTED ANSWERS:             343 TO     1049

L2            2 SEA SSS SAM L1

=> search l1
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 04:40:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   699751 TO ITERATE

100.0% PROCESSED   699751 ITERATIONS                              1206 ANSWERS
SEARCH TIME: 00.00.03

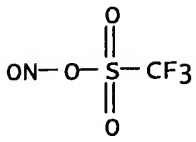
L3         1206 SEA SSS FUL L1

=> s triflate
L4          791 TRIFLATE

=> d l4 780-791

L4   ANSWER 780 OF 791  REGISTRY  COPYRIGHT 2006 ACS on STN
RN   14848-27-2  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Methanesulfonic acid, trifluoro-, anhydride with nitrous acid (9CI)  (CA
     INDEX NAME)
OTHER CA INDEX NAMES:
CN   Methanesulfonyl nitrite, trifluoro- (8CI)
OTHER NAMES:
CN   Nitrosonium triflate
CN   Trifluoromethanesulfonyl nitrite
MF   C F3 N O4 S
```

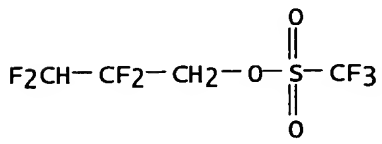
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAPLUS, CASREACT, CHEMINFORMRX
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 781 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 6401-02-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, 2,2,3,3-tetrafluoropropyl ester (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanol, 2,2,3,3-tetrafluoro-, trifluoromethanesulfonate (8CI)
OTHER NAMES:
CN 2,2,3,3-Tetrafluoropropan-1-yl triflate
CN 2,2,3,3-Tetrafluoropropyl trifluoromethanesulfonate
MF C4 H3 F7 O3 S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)

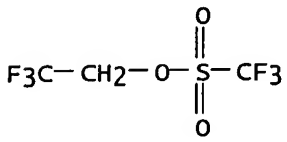


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)
14 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 782 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 6226-25-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, 2,2,2-trifluoroethyl ester (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethanol, 2,2,2-trifluoro-, trifluoromethanesulfonate
OTHER NAMES:
CN 2,2,2-Trifluoroethyl triflate
CN 2,2,2-Trifluoroethyl trifluoromethanesulfonate
CN 2,2,2-Trifluoroethyl trifluoromethylsulfonate
CN Trifluoromethanesulfonic acid 2,2,2-trifluoroethyl ester
MF C3 H2 F6 O3 S

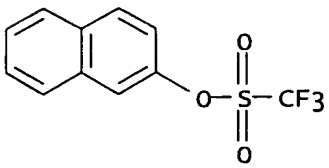
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, IFICDB, IFIPAT, IFIUDB, PS, RTECS*, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

164 REFERENCES IN FILE CA (1907 TO DATE)
165 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 783 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 3857-83-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, 2-naphthalenyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Naphthol, trifluoromethanesulfonate (8CI)
CN Methanesulfonic acid, trifluoro-, 2-naphthyl ester (7CI, 8CI)
OTHER NAMES:
CN β-Naphthyl triflate
CN 2-((Trifluoromethanesulfonyl)oxy)naphthalene
CN 2-Naphthalenyl triflate
CN 2-Naphthyl triflate
CN 2-Naphthyl trifluoromethanesulfonate
MF C11 H7 F3 O3 S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, USPAT2, USPATFULL
(*File contains numerically searchable property data)

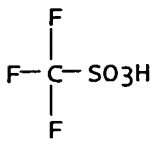


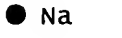
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

122 REFERENCES IN FILE CA (1907 TO DATE)
122 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 784 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 2926-30-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, sodium salt (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Sodium triflate

CN Sodium trifluoromethanesulfonate
CN Sodium trifluoromethylsulfonate
CN Trifluoromethanesulfonic acid sodium salt
MF C H F3 O3 S . Na
CI COM
LC STN Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
CRN (1493-13-6)

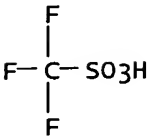




PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

411 REFERENCES IN FILE CA (1907 TO DATE)
36 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
412 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 785 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 2926-27-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, potassium salt (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Potassium triflate
CN Potassium trifluoromethanesulfonate
CN Potassium trifluoromethylsulfonate
CN Trifluoromethanesulfonic acid potassium salt
DR 32578-37-3
MF C H F3 O3 S . K
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
CRN (1493-13-6)

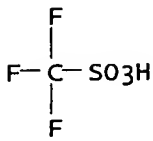


● K

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

199 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
199 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 786 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 2923-28-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, silver(1+) salt (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Silver (trifluoromethyl)sulfonate
CN Silver triflate
CN Silver trifluoromethanesulfonate
CN Silver trifluoromethanesulphonate
CN Silver(1+) triflate
CN Silver(1+) trifluoromethanesulfonate
CN Silver(I) triflate
CN Silver(I) trifluoromethanesulfonate
CN Trifluoromethanesulfonic acid silver(1+) salt
DR 499776-24-8, 637342-85-9, 330649-44-0, 380240-12-0, 460355-11-7
MF C H F3 O3 S . Ag
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, MSDS-OHS, PROMT, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (1493-13-6)

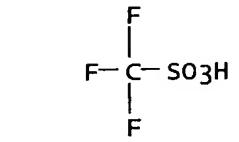


● Ag(I)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1272 REFERENCES IN FILE CA (1907 TO DATE)
35 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1277 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 787 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 2794-60-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, barium salt (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Barium bis(trifluoromethanesulfonate)
CN Barium triflate
CN Barium triflate (Ba(CF3SO3)2)
CN Barium trifluoromethanesulfonate
MF C H F3 O3 S . 1/2 Ba
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
CRN (1493-13-6)



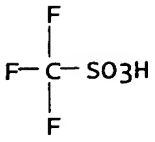
●1/2 Ba

51 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
52 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 788 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 591-40-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, compd. with benzenamine (1:1) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzenamine, trifluoromethanesulfonate (9CI)
CN Methanesulfonic acid, trifluoro-, compd. with aniline (1:1) (8CI)
CN Methanesulfonic acid, trifluoro-, PhNH2 salt (6CI)
OTHER NAMES:
CN Anilinium triflate
CN Anilinium trifluoromethanesulfonate
MF C6 H7 N . C H F3 O3 S
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB, USPATFULL
(*File contains numerically searchable property data)

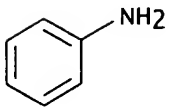
CM 1

CRN 1493-13-6
CMF C H F3 O3 S



CM 2

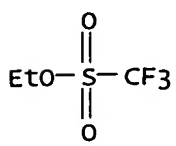
CRN 62-53-3
CMF C6 H7 N



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

11 REFERENCES IN FILE CA (1907 TO DATE)
11 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

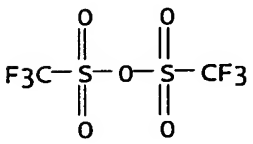
L4 ANSWER 789 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 425-75-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl triflate
CN Ethyl trifluoromethanesulfonate
CN Ethyl trifluoromethylsulfonate
CN Trifluoromethanesulfonic acid ethyl ester
MF C3 H5 F3 O3 S
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

197 REFERENCES IN FILE CA (1907 TO DATE)
197 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 790 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 358-23-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, anhydride (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Perfluoromethanesulfonic anhydride
CN Tirflic anhydride
CN Triflate anhydride
CN Triflic acid anhydride
CN Triflic anhydride
CN Trifluoromethanesulfonic acid anhydride
CN Trifluoromethanesulfonic anhydride
CN Trifluoromethylsulfonic acid anhydride
CN Trifluoromethylsulfonic anhydride
DR 93916-16-6
MF C2 F6 O5 S2
CI COM
LC STN Files: BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, IPA, MSDS-OHS, PIRA, PROMT, PS, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

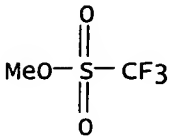


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2021 REFERENCES IN FILE CA (1907 TO DATE)
10 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2026 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 791 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
RN 333-27-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Methanesulfonic acid, trifluoro-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN Methyl triflate
CN Methyl trifluoromethanesulfonate
CN NSC 270679
CN Trifluoromethanesulfonic acid methyl ester
MF C2 H3 F3 O3 S
CI COM
LC STN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, MEDLINE, PIRA, PROMT, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL

(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

909 REFERENCES IN FILE CA (1907 TO DATE)
17 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
911 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

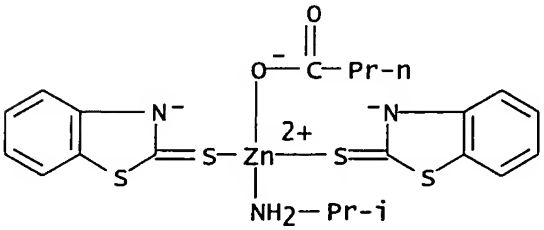
=> d his

(FILE 'HOME' ENTERED AT 04:28:36 ON 11 DEC 2006)

FILE 'REGISTRY' ENTERED AT 04:39:37 ON 11 DEC 2006
L1 STRUCTURE UPLOADED
L2 2 S L1
L3 1206 SEARCH L1 FULL
L4 791 S TRIFLATE

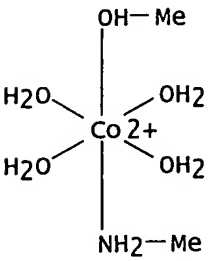
=> d l3 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200

L3 ANSWER 100 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 765886-51-9 REGISTRY
ED Entered STN: 20 Oct 2004
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C21 H24 N3 O2 S4 Zn
CI CCS, COM
SR CA



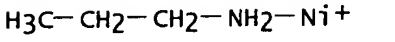
L3 ANSWER 200 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 282549-07-9 REGISTRY
ED Entered STN: 02 Aug 2000
CN Cobalt(2+), tetraaqua(methanamine)(methanol)-, (OC-6-32)- (9CI) (CA INDEX NAME)
MF C2 H17 Co N O5

CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 300 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 149641-87-2 REGISTRY
ED Entered STN: 27 Aug 1993
CN Nickel(1+), (1-propanamine)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (Propylamine)nickel(1+)
MF C3 H9 N Ni
CI CCS
SR CA
LC STN Files: CA, CAPLUS

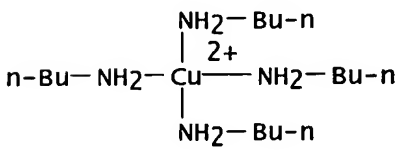


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 400 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 132517-77-2 REGISTRY
ED Entered STN: 08 Mar 1991
CN Copper(2+), tetrakis(1-butanamine)-, diperchlorate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex
MF C16 H44 Cu N4 . 2 Cl O4
SR CA
LC STN Files: CA, CAPLUS

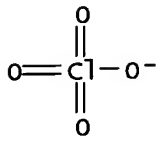
CM 1

CRN 30904-66-6
CMF C16 H44 Cu N4
CCI CCS



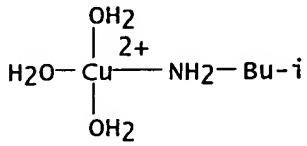
CM 2

CRN 14797-73-0
CMF Cl O4



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 500 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 110303-66-7 REGISTRY
ED Entered STN: 19 Sep 1987
CN Copper(2+), triaqua(2-methyl-1-propanamine)-, (SP-4-2)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, 2-methyl-, copper complex
MF C4 H17 Cu N O3
CI CCS, COM
SR CA



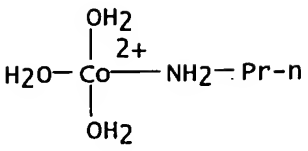
L3 ANSWER 600 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 91172-12-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt(2+), triaqua(1-propanamine)-, (T-4)-, (OC-6-22)-pentakis(cyano-C)nitrosylferrate(2-) (1:1), trihydrate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, cobalt complex
CN Ferrate(2-), pentakis(cyano-C)nitrosyl-, (OC-6-22)-, (T-4)-triaqua(1-propanamine)cobalt(2+) (1:1), trihydrate (9CI)
MF C5 Fe N6 O . C3 H15 Co N O3 . 3 H2 O
LC STN Files: CA, CAPLUS

CM 1

CRN 91172-11-1
CMF C5 Fe N6 O . C3 H15 Co N O3

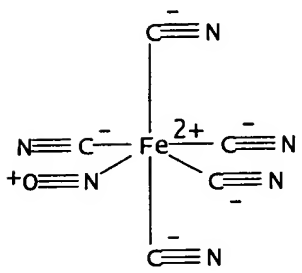
CM 2

CRN 91172-10-0
CMF C3 H15 Co N O3
CCI CCS



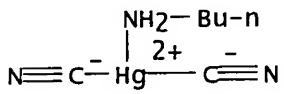
CM 3

CRN 15078-28-1
CMF C5 Fe N6 O
CCI CCS



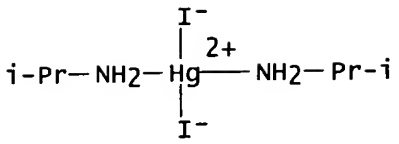
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 700 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 68245-50-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Mercury, (1-butanamine)bis(cyano-C)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, mercury complex
MF C6 H11 Hg N3
CI CCS
LC STN Files: CA, CAPLUS



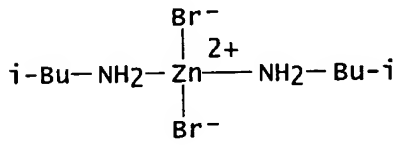
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 800 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 56873-03-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Mercury, diiodobis(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Propanamine, mercury complex
OTHER NAMES:
CN Mercuric iodide compound with isopropylamine (1:2)
MF C6 H18 Hg I2 N2
CI CCS
LC STN Files: CA, CAPLUS



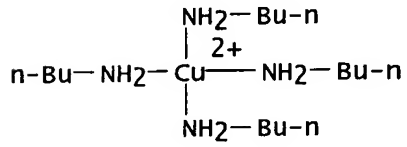
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 900 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 40231-90-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Zinc, dibromobis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, 2-methyl-, zinc complex
MF C8 H22 Br2 N2 Zn
CI CCS
LC STN Files: CA, CAPLUS



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

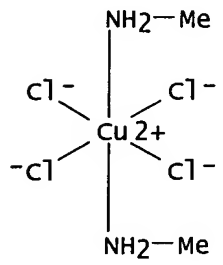
L3 ANSWER 1000 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 30904-66-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper(2+), tetrakis(1-butanamine)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex
CN Copper(2+), tetrakis(butylamine)-, ion (8CI)
OTHER NAMES:
CN Tetrakis(butylamine)copper(2+)
CN Tetrakis(butylamine)copper(II)
MF C16 H44 Cu N4
CI CCS, COM
LC STN Files: CA, CAPLUS, GMELIN*
(*File contains numerically searchable property data)



3 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 1100 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 18901-59-2 REGISTRY

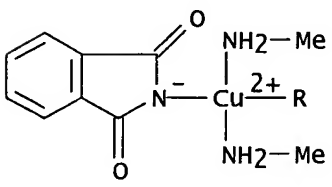
ED Entered STN: 16 Nov 1984
CN Cuprate(2-), tetrachlorobis(methylamine)-, dihydrogen (8CI) (CA INDEX NAME)
MF C2 H10 Cl4 Cu N2 . 2 H
CI CCS
LC STN Files: CA, CAPLUS
CRN (795219-69-1)

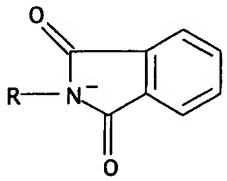


● 2 H^+

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 1200 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 13987-19-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(methylamine)bis(phthalimidato)- (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Copper, bis(phthalimidato)bis(methylamine)- (7CI)
MF C18 H18 Cu N4 O4
CI CCS
LC STN Files: CA, CAOLD, CAPLUS



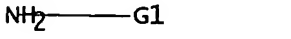


5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

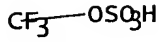
=>
Uploading C:\Program Files\Stnexp\Queries\10749450a.str

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G2



G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu
G2 Ag,Cd,Co,Cu,Fe,Hg,Ni,Zn

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 04:47:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

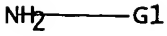
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=>
Uploading C:\Program Files\Stnexp\Queries\10749450b.str

L7 STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7 STR



G2

G3

G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G2 Ag,Cd,Co,Cu,Fe,Hg,Ni,Zn

G3 S,P

Structure attributes must be viewed using STN Express query preparation.

```
=> s l7
SAMPLE SEARCH INITIATED 04:49:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    11364 TO ITERATE

 17.6% PROCESSED     2000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       220892 TO   233668
PROJECTED ANSWERS:               0 TO        0

L8            0 SEA SSS SAM L7

=> search l7
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 04:49:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   228829 TO ITERATE

100.0% PROCESSED   228829 ITERATIONS                              121 ANSWERS
SEARCH TIME: 00.00.01

L9          121 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   390.84     394.62

FILE 'CAPLUS' ENTERED AT 04:49:41 ON 11 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 11 Dec 2006 VOL 145 ISS 25
FILE LAST UPDATED: 10 Dec 2006 (20061210/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l9
L10 46 L9

=> d l10 fbib ab hitstr 1-46

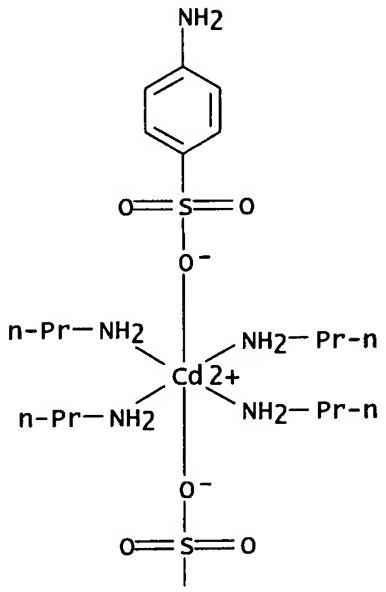
L10 ANSWER 1 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:344669 CAPLUS
DN 141:81204
TI Reversible and selective amine interactions of [Cd(μ2-N,O-p-NH2C6H4SO3)2(H2O)2]n
AU Zhou, Jin-Sen; Cai, Jiwen; Wang, Li; Ng, Seik-Weng
CS School of Chemistry & Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, Peop. Rep. China
SO Dalton Transactions (2004), (9), 1493-1497
CODEN: DTARAF; ISSN: 1477-9226
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 141:81204
AB [Cd(μ2-N,O-p-NH2C6H4SO3)2(H2O)2]n (1) is a layered coordination compound The solid-vapor reactions between crystalline 1 and volatile amines were studied and the corresponding amine adducts were characterized by elemental anal., TGA, PXRD and IR. Among them, the C2H5NH2 and PrNH2 adducts, [Cd(C2H5NH2)4(H2O)2](H2NC6H4SO3)2 (3) and [Cd(PrNH2)4(O-p-H2NC6H4SO3)2]·PrNH2 (4), grew into single crystals in situ from the solid-vapor reaction processes and their crystal structures were characterized. In both cases, 4 mol equivalent of amine mols. coordinate to Cd(II) via replacing the N,O-p-NH2C6H4SO3 ligands or coordinated H2O mols. The single-phase product suggests that the solid-vapor reaction between the metal sulfonate and volatile alkylamines could be used as a green process to synthesize monoamine-coordinated Cd(II) complexes without any solvent and routine separation Finally, the substitution reaction is reversible at room conditions and selective for primary alkylamines.
IT 713079-80-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation via reversible solid-vapor coordinative substitution of layered cadmium(II) aminobenzenesulfonate aqua complex solid with volatile alkylamine, and crystal structure and TGA of)

RN 713079-80-2 CAPLUS
CN Cadmium, bis(4-aminobenzenesulfonato-κO)tetrakis(1-propanamine)-, (OC-6-12)-, compd. with 1-propanamine (1:1) (9CI) (CA INDEX NAME)

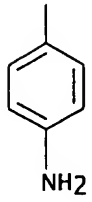
CM 1

CRN 713079-79-9
CMF C24 H48 Cd N6 O6 S2
CCI CCS

PAGE 1-A

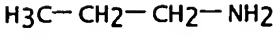


PAGE 2-A



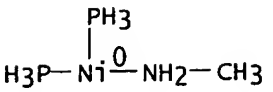
CM 2

CRN 107-10-8
CMF C3 H9 N

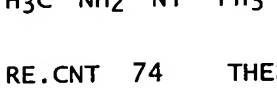


RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:613865 CAPLUS
DN 140:357466
TI Theoretical studies on C-heteroatom bond formation via reductive elimination from group 10 M(PH3)2(CH3)(X) species (X = CH3, NH2, OH, SH) and the determination of metal-X bond strengths using density functional theory
AU MacGregor, Stuart A.; Neave, Greg W.; Smith, Christopher
CS Department of Chemistry, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK
SO Faraday Discussions (2003), 124, 111-127
CODEN: FDISE6; ISSN: 1359-6640
PB Royal Society of Chemistry
DT Journal
LA English
AB D. functional calcns. were used to investigate C-C, C-N and C-O bond forming reactions via reductive elimination from Group 10 cis-[M(PH3)2(Me)(X)] species (X = Me, NH2, OH). Both direct reaction from the four-coordinate species and a three-coordinate mechanism involving initial PH3 loss was considered. For the four-coordinate pathway the ease of reductive elimination to give M(PH3)2 and Me-X follows the trend M = Pd < Pt < Ni. The reaction of the cis-M(PH3)2(Me)(NH2) species is promoted by the formation of methylamine adducts. Non-planar transition states are located and the C-heteroatom bond forming processes are characterized by migration of Me onto the cis-heteroatom ligand. For a given ligand, X, activation energies follow the trend M = Ni < Pd < Pt. Formation of the three-coordinate M(PH3)(Me)(X) species is promoted by a labilization of the cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OH. For the three-coordinate pathway the energy change for reductive elimination to give M(PH3) and Me-X again follows the trend M = Pd < Pt < Ni and in all cases the initial product is an M(PH3)(XMe) adduct. The three-coordinate transition states again involve migration of the Me ligand onto the cis-X ligand and for X = NH2 or OH activation energies follow the trend Ni > Pd < Pt. For a given metal activation energies in both the four- and three-coordinate pathways increase along the series Me < NH2 < OH. These trends in activation energy can be rationalized in terms of the strength of M-Me/M-X bonding as long as the extent of geometrical distortion required to obtain the transition state geometry is taken into account. Further calcns. on cis-Pd(PH3)2(Me)(SH) suggest that the more common exptl. observation of C(sp3)-S compared to C(sp3)-O reductive elimination arises from the greater kinetic accessibility of the former process rather than an intrinsic thermodn. preference for C-S bond formation. By comparison, the calcns. indicate that C(sp3)-N reductive elimination should be feasible from Ni and Pd systems. DF calcns. are shown to reproduce the relative homolytic bond strengths determined exptl. for Pt-X bonds. In the cis-M(PH3)2(Me)(X) systems the M-Me homolytic bond strength increases down the group while for M-NH2 and M-OH bonds the trend is M = Ni ≈ Pd < Pt. M-NH2 and M-OH bonds are considerably stronger than M-Me bonds and the presence of a heteroatom ligand serves to weaken M-CH3 bonds even further.
IT 682767-97-1, (Methanamine)bis(phosphine)nickel
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(optimized geometry, potential energy, dissociation; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)
RN 682767-97-1 CAPLUS
CN Nickel, (methanamine)bis(phosphine)- (9CI) (CA INDEX NAME)



IT 682768-13-4, (Methanamine)(phosphine)nickel
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)
RN 682768-13-4 CAPLUS
CN Nickel, (methanamine)(phosphine)- (9CI) (CA INDEX NAME)



RE.CNT 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:509917 CAPLUS
DN 139:77881
TI Metal thioether complexes as organic metal precursors for use in forming metal-containing patterned films
IN Jung, Won Cheol; Chang, Seok; Hwang, Soon Taik; Byun, Young Hun
PA Samsung Electronics Co., Ltd., S. Korea
SO Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

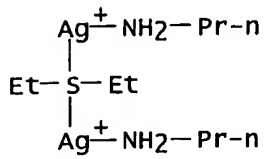
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP 1323721	A2	20030702	EP 2002-257784	20021111
EP 1323721	A3	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
			KR 2001-87510	A 20011228
KR 2003057133	A	20030704	KR 2001-87510	20011228
US 2003124457	A1	20030703	US 2002-282031	20021029
US 6965045	B2	20051115		
			KR 2001-87510	A 20011228
JP 2003286579	A2	20031010	JP 2002-373621	20021225
			KR 2001-87510	A 20011228

OS MARPAT 139:77881
AB Disclosed are organic metal precursors comprising one or more thioether ligands bonded to one or more metal atoms (metal = Ag, Au, Co, Cu, Pd, Ni, Pt, Zn, Cd), wherein the organic ligand is rapidly dissociated from the metal atom upon exposure to light and degraded leaving a metal or a metal oxide. Thus, reaction of AgNO2 and Et2S in heated MeCN afforded [(Et2S)Ag+](NO2-). Reaction of the latter with PrNH2 in MeCN afforded [(PrNH2)Ag]2SEt2. Using the organic metal precursors of the present invention, e.g., [(PrNH2)Ag]2SEt2, an electroconductive, metal-containing patterned film can be easily deposited on a substrate at room temperature under atmospheric pressure without using photosensitive resins.
IT 550305-04-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation as precursor for use in forming metal-containing patterned film via
photodegrdn. without use of photosensitive resins)
RN 550305-04-9 CAPLUS
CN Silver(2+), bis(1-propanamine)[μ-[1,1'-thiobis[ethane]]]di-, dinitrite (9CI) (CA INDEX NAME)

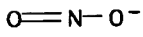
CM 1

CRN 550305-03-8
CMF C10 H28 Ag2 N2 S
CCI CCS



CM 2

CRN 14797-65-0
CMF N O2



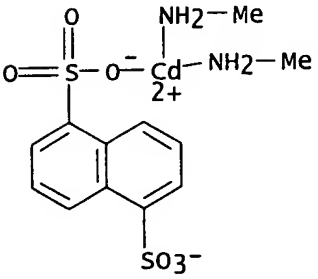
L10 ANSWER 4 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:472276 CAPLUS
DN 139:239001
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.

IT 595548-10-0P 595548-12-2P 595548-14-4P
595548-16-6P 595548-18-8P 595548-20-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)

RN 595548-10-0 CAPLUS
CN Cadmium, bis(methanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with methanamine (1:1), dihydrate (9CI) (CA INDEX NAME)

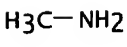
CM 1

CRN 595548-09-7
CMF C12 H16 Cd N2 O6 S2
CCI CCS



CM 2

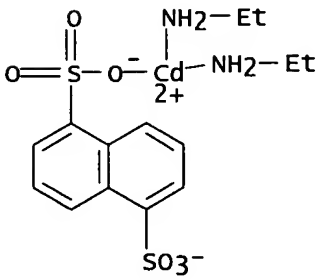
CRN 74-89-5
CMF C H5 N



RN 595548-12-2 CAPLUS
CN Cadmium, bis(ethanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with ethanamine (1:2), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 595548-11-1
CMF C14 H20 Cd N2 O6 S2
CCI CCS



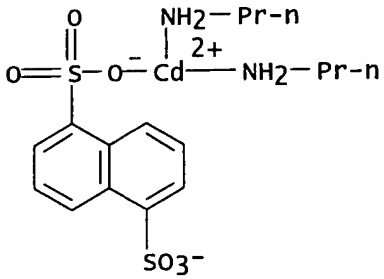
CM 2

CRN 75-04-7
CMF C2 H7 N

RN 595548-14-4 CAPLUS
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(1-propanamine)-, compd. with 1-propanamine (1:2), dihydrate (9CI) (CA INDEX NAME)

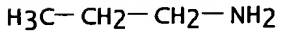
CM 1

CRN 595548-13-3
CMF C16 H24 Cd N2 O6 S2
CCI CCS



CM 2

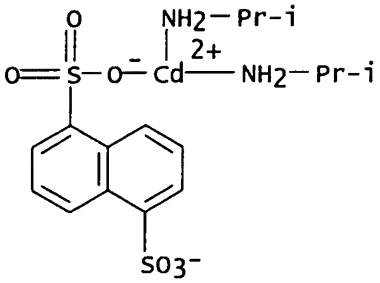
CRN 107-10-8
CMF C3 H9 N



RN 595548-16-6 CAPLUS
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(2-propanamine)-, compd. with 2-propanamine (1:1), dihydrate (9CI) (CA INDEX NAME)

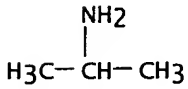
CM 1

CRN 595548-15-5
CMF C16 H24 Cd N2 O6 S2
CCI CCS



CM 2

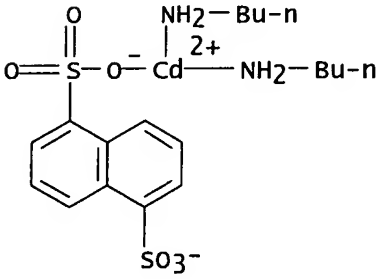
CRN 75-31-0
CMF C3 H9 N



RN 595548-18-8 CAPLUS
CN Cadmium, bis(1-butanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with 1-butanamine (1:1), dihydrate (9CI) (CA INDEX NAME)

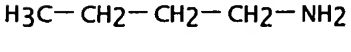
CM 1

CRN 595548-17-7
CMF C18 H28 Cd N2 O6 S2
CCI CCS



CM 2

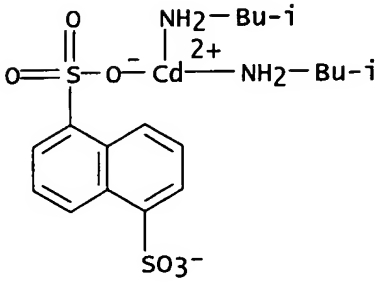
CRN 109-73-9
CMF C4 H11 N



RN 595548-20-2 CAPLUS
CN Cadmium, bis(2-methyl-1-propanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with 2-methyl-1-propanamine (1:1), dihydrate (9CI) (CA INDEX NAME)

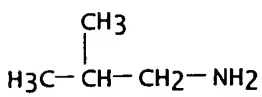
CM 1

CRN 595548-19-9
CMF C18 H28 Cd N2 O6 S2
CCI CCS



CM 2

CRN 78-81-9
CMF C4 H11 N



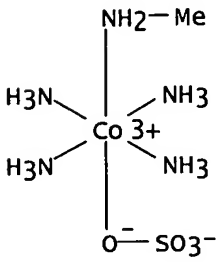
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2002:283881 CAPLUS
DN 137:84151
TI Activation volumes for a series of spontaneous, acid-and base-catalysed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-)
AU Benzo, Fabian; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz
CS Catedra de Quimica Inorganica, Facultad de Quimica, Universidad de la Republica, Montevideo, 11800, Urug.
SO Inorganic Reaction Mechanisms (Amsterdam, Netherlands) (2001), 3(1), 25-29
CODEN: IRMEFE; ISSN: 1028-6624
PB Gordon & Breach Science Publishers
DT Journal
LA English
AB The vols. of activation for the spontaneous, base-, and acid- catalyzed path of the hydrolysis reaction of a series of trans-[Co(MeNH2)(NH3)4X](3-n)+ ions (X = Cl-, Br-, (ONO2)- (OSO3)2-) have been determined in order to establish analogies with the dissociative trends found in previous work with the spontaneous hydrolysis of neutral ligands from the same cores. While for the base catalyzed path a significant decrease in the activation volume is found on going from the {Co(NH3)5} to the trans-{Co(MeNH2)(NH3)4} inert skeleton (i.e. 9.8, 12.5, 4.0 and 9.1 cm3mol-1 for the chloro, bromo, nitrato and sulfato derivs.), no significant changes are observed for the same complexes in the spontaneous reaction. The trends are rationalized in terms of the important changes occurring in electrostriction factors for the DCB and Id intimate mechanisms operating

and the important increase in the degree of dissociativeness due to the presence of a trans-methylamino ligand. For the acid catalyzed path the differences are much more difficult to assess, specially taking into account the limited information available as well as the inherent errors involved in the rate constant determination

IT 210574-34-8
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-))

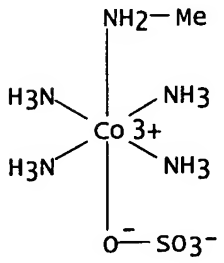
RN 210574-34-8 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κO]-, (OC-6-23)-(9CI) (CA INDEX NAME)



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:445849 CAPLUS
DN 133:49533
TI Aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobalt(III) complex ion
AU Benzo, Fabian; Capparelli, Alberto L.; Martire, Daniel O.; Sienra, Beatriz
CS Catedra de Quimica Inorganica, Facultad de Quimica, Montevideo, C.C.1157, Urug.
SO Inorganic Reaction Mechanisms (Amsterdam) (2000), 1(4), 319-324
CODEN: IRMEFE; ISSN: 1028-6624
PB Gordon & Breach Science Publishers
DT Journal
LA English
AB The kinetics of aquation and base hydrolysis reactions of trans-[Co(NH3)4(NH2CH3)(OSO3)]+ have been studied. In acid solution the aquation rate, Raq, follows the equation Raq/[complex] = ks + kc[H+], at constant ionic strength μ = 1.0 M. The activation parameters are ΔHs# = 88.8 kJ mol-1, ΔSs# = -50.5 JK-1 mol-1, ΔHc# = 96.7 kJ mol-1 and ΔSc# = -23 JK-1 mol-1. The rate consts. at 25°C are ks = 4.15 + 10-6 s-1 and kc = 4.52 M-1 s-1. The rate of base hydrolysis, ROH, follows the equation ROH/[complex] = kOH [OH-]. The activation parameters are ΔHOH# = 74.9 kJmol-1 and ΔSOH# = 2JK-1 mol-1 and the rate constant is kOH = 0.58 M-1 s-1 at 25°C and μ = 0.15 M. The stereochem. of the hydroxo product has been determined (cis-[Co(NH3)4(NH2CH3)-(OH)]2+ = 9%). The results are discussed in the light of the reaction mechanisms proposed so far.
IT 210574-34-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatoc
obalt(III) complex ion)
RN 210574-34-8 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κO]-, (OC-6-23)-
(9CI) (CA INDEX NAME)

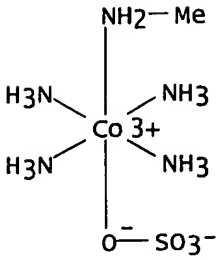


RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:398528 CAPLUS
DN 133:79995
TI Inductive effect of methyl groups on acidopentaaminecobalt(III) complexes
AU Benzo, Fabian; Beyer, Lothar; Bozoglian, Fernando; Hallmeier, Karl-Heinz;
Sienra, Beatriz
CS Universidad de la Republica, Catedra de Quimica Inorganica, Montevideo,
Urug.
SO Polyhedron (2000), 19(8), 971-974
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
AB Electron spectroscopy for chemical anal. (ESCA) was performed for
[Co(NH3)5Cl](Clo4)2, trans-[Co(NH3)4(NH2CH3)Cl]-(Clo4) 2,
[Co(NH2CH3)5Cl](Clo4)2 and trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl 04)
complexes. Comparison of the results for the complexes
[Co(NH3)5Cl](Clo4)2 and trans-[Co(NH3)4(NH2CH3)Cl](Clo4)2 shows clearly
the electronic influence (+I effect) of the methylamine group on the
cobalt and through this on the chlorine atom in trans position.
Comparison of [Co(NH2CH3)5Cl](Clo4)2 with trans-
[Co(NH3)4(NH2CH3)Cl](Clo4)2 shows that methylation of the four cis-NH3
ligands does not produce a proportional decrease in the binding energy of
the cobalt atom, while the electron d. of the chloro ligand is not
affected. For the complex trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl 04) the +I
effect is almost completely compensated by the presence of the sulfato
group in trans position. Acid dissociation consts. are also reported for
[Co(NH3)5(OH2)]3+ and trans-[Co(NH3)4(NH2CH3)(OH2)]3 + ions. The
implications of these results for the mechanism of the acid and base
hydrolysis reactions of acidopentaaminecobalt(III) complexes are
discussed. The preparation of the trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl 04)
complex through the trans-[Co(NH3)4(NH2CH3)(SO3)]+ precursor is also
described.
IT 279674-00-9
RL: PRP (Properties)
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
RN 279674-00-9 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κO]-, (OC-6-23)-,
perchlorate (9CI) (CA INDEX NAME)

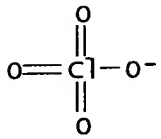
CM 1

CRN 210574-34-8
CMF C H17 Co N5 O4 S
CCI CCS

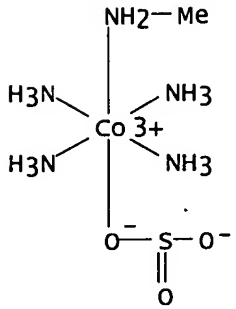


CM 2

CRN 14797-73-0
CMF Cl O4



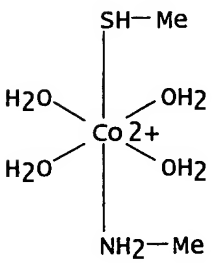
IT 134066-32-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(inductive effect of Me groups on acidopentaamminecobalt(III) complexes)
RN 134066-32-3 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-κO]-, (OC-6-23)-
(9CI) (CA INDEX NAME)



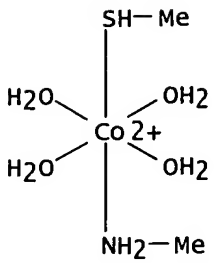
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:22952 CAPLUS

DN 133:125569
TI Ab Initio calculations of [CoY6-nXn]2+ complexes
AU Rulisek, Lubomir; Havlas, Zdenek
CS Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic, Prague, 166 10, Czech Rep.
SO Journal of Chemical Physics (2000), 112(1), 149-157
CODEN: JCPSA6; ISSN: 0021-9606
PB American Institute of Physics
DT Journal
LA English
AB The CASSCF and multi-reference second order perturbation theory (CASPT2) calcns. of [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes (X = CH3OH, CH3SH, CH3NH2) are reported. The potential energy surfaces of 10 lowest quartet states of [Co(H2O)5X]2+ complexes near the equilibrium geometry are calculated and splitting of triple-degenerate 4T1g(F), 4T2g(F), and 4T1g(P) electronic states of [Co(H2O)6]2+ complex induced by the substitution of one or two water ligands is characterized and quantified. The energy differences between originally degenerate states are almost invariant to the changes of metal-ligand distances, and despite their proximity, the crossing does not occur. The coeffs. of the leading configuration of multi-reference wave functions of [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes are shown to approach unity and the usage of single-reference methods is justified. As a consequence, interaction energies of the studied functional groups with Co2+ are computed also at the HF, DFT and MP2 levels. They are compared to CASSCF calcns. and to the equivalent calcns. done for Zn2+ and Ni2+ ions. The computational methodol. for the accurate calcns. of various cobalt (II) ionic complexes is described and the implications for the theor. investigation of interactions of chemical and biol. important functional groups with Co2+ are discussed.
IT 282547-96-0 284476-55-7
RL: PRP (Properties)
(ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))
RN 282547-96-0 CAPLUS
CN Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-32)- (9CI) (CA INDEX NAME)



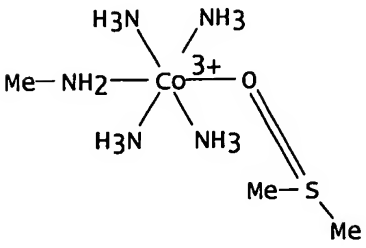
RN 284476-55-7 CAPLUS
CN Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-23)- (9CI) (CA INDEX NAME)



RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

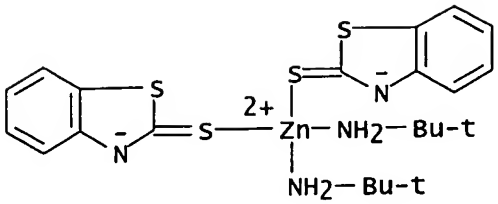
L10 ANSWER 9 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:759418 CAPLUS
DN 132:142592
TI Variable temperature and pressure study of the aquation reactions of cobalt(III) and chromium(III) penta- and tetra-amines
AU Benzo, Fabian; Bernhardt, Paul V.; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz
CS Facultad de Quimica, Catedra de Quimica Inorganica, Universidad de la Republica, Montevideo, 11800, Urug.
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (22), 3973-3979
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
AB Preparation of a series of specific penta- and tetra-amine derivs. of CoIII and CrIII with a neutral leaving ligand has been carried out in order to accomplish a fine tuning of the associativeness/dissociativeness of their substitution reactions. Spontaneous aquation reactions of the neutral ligands have been studied at variable temperature and pressure. Although rate consts. and thermal activation parameters show an important degree of scatter, the values determined for the activation vols. of the substitution process illustrate the mechanistic fine tuning that may be achieved for these reactions. In all cases, in the absence of important steric constraints in the mol., electronic inductive effects seem to be the most important factor accounting for the dissociative shifts observed both for pentaamine i.e. ΔV.dbldag. = +4.0 or +14.0 cm3 mol-1 and +5.2 or +16.5 cm3 mol-1 for the aquation of cis- or trans-[Co(MeNH2)(NH3)4(DMF)]3+ and cis- or trans-[CoL15(DMF)]3+ resp., where L15 represents a pentaamine macrocyclic ligand, tetraamine systems i.e. ΔV.dbldag. = +4.1 or +8.4 cm3 mol-1 and -10.8 or -7.4 cm3 mol-1 for the aquation of cis-[Co(NH3)4Cl(DMAC)]2+ (DMAC = dimethylacetamide) or cis-[Co(en)2Cl(DMAC)]2+ and cis-[Cr(NH3)4Cl(DMF)]2+ or cis-[Cr(en)2Cl(DMF)]2+. From the results, clear evidence is obtained which indicates that, only when the situation is borderline Ia/Id, or the steric demands are increased dramatically, dissociative shifts are observed; in all other cases electronic inductive effects seem to be dominant for such a tuning of the substitution process.
IT 138521-43-4
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(variable temperature and pressure study of aquation reactions of cobalt(III) and chromium(III) penta- and tetra-amines)
RN 138521-43-4 CAPLUS
CN Cobalt(3+), tetraammine(methanamine)[(sulfinyl-κO)bis[methane]]-,

(OC-6-23)- (9CI) (CA INDEX NAME)

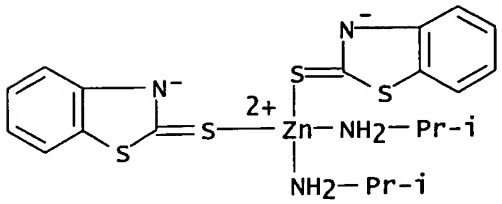


RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

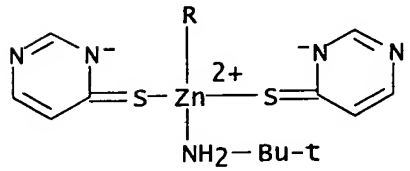
L10 ANSWER 10 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:702066 CAPLUS
DN 132:36842
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
AB Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
IT 15214-57-0 252564-24-2 252564-26-4
252564-27-5 252564-28-6 252564-30-0
252564-31-1 252564-34-4 252564-35-5
252564-36-6 252564-37-7 252564-38-8
252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
RN 15214-57-0 CAPLUS
CN Zinc, bis(2(3H)-benzothiazolethionato-κS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

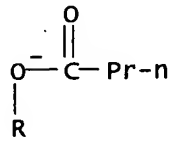


RN 252564-24-2 CAPLUS
CN Zinc, bis(2(3H)-benzothiazolethionato-κS2)bis(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

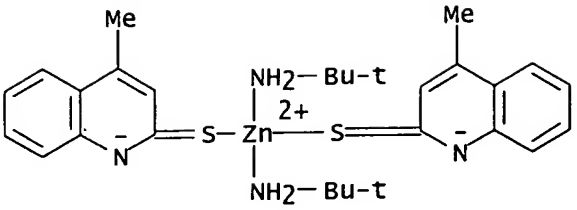


RN 252564-26-4 CAPLUS
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4(1H)-pyrimidinethionato-κS4)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

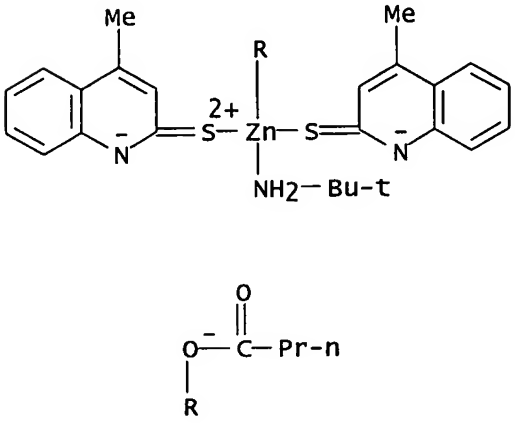




RN 252564-27-5 CAPLUS
CN Zinc, bis(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)

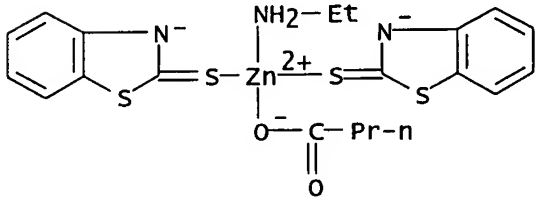


RN 252564-28-6 CAPLUS
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



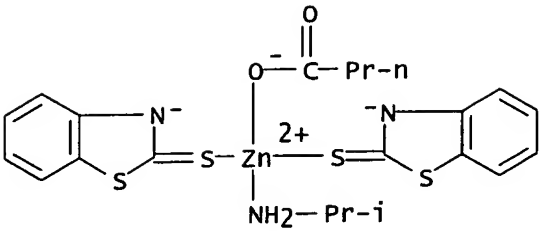
● H+

RN 252564-30-0 CAPLUS
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(ethanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



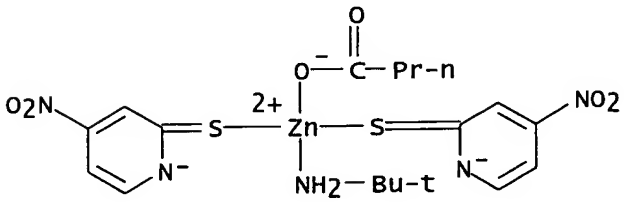
● H+

RN 252564-31-1 CAPLUS
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



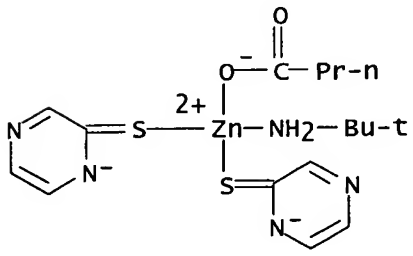
● H^+

RN 252564-34-4 CAPLUS
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4-nitro-2(1H)-pyridinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



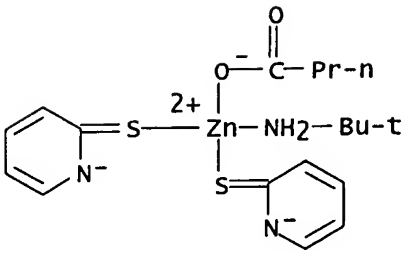
● H^+

RN 252564-35-5 CAPLUS
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyrazinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



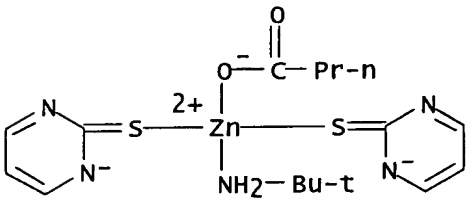
● H^+

RN 252564-36-6 CAPLUS
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyridinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



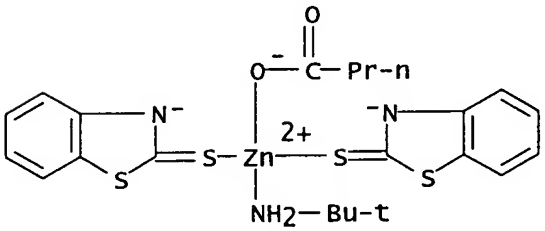
● H^+

RN 252564-37-7 CAPLUS
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyrimidinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



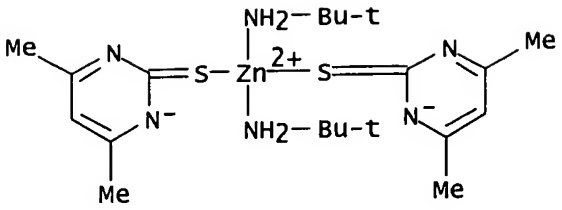
● H^+

RN 252564-38-8 CAPLUS
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-methyl-2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)



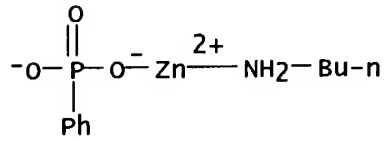
● H^+

RN 252564-83-3 CAPLUS
CN Zinc, bis(4,6-dimethyl-2(1H)-pyrimidinethionato-κS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

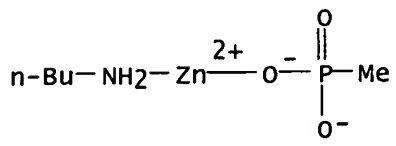


RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1999:645540 CAPLUS
DN 132:8432
TI An organometallic route to zinc phosphonates and their intercalates
AU Gerbier, Philippe; Guerin, Christian; Henner, Bernard; Unal, Jean-Remi
CS U.M.R. 5637 -Universite Montpellier II, Montpellier, 34095, Fr.
SO Journal of Materials Chemistry (1999), 9(10), 2559-2565
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
AB An organometallic nonaq. route to zinc phosphonates and to their intercalates was studied. Various phosphonic acids react with dimethylzinc in THF media to afford the corresponding layered zinc phosphonates Zn(O3PR1) (R1 = Me, Ph, 2- and 3-thienyl, thiophen-3-ylmethyl) with evolution of methane. The presence of a primary n-alkylamine in the reaction mixture allows the 1-pot formation of 2-dimensional-layered intercalated phases Zn(O3PR1)·RNH2 [R2 = Bu, Penn (n-pentyl)] whereas a more bulky amine such as cyclohexylamine (HexcNH2) give 1-dimensional polymeric chains Zn(O3PPh)·2HexcNH2.
IT 162050-26-2P 184824-62-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectrum of intercalate)
RN 162050-26-2 CAPLUS
CN Zinc, (1-butanamine)[phenylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)

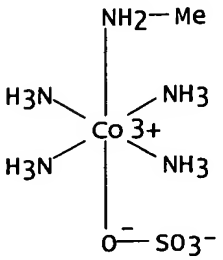


RN 184824-62-2 CAPLUS
CN Zinc, (1-butanamine)[methylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)



RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 12 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1998:433445 CAPLUS
DN 129:141178
TI Competition study for the base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ complexes
AU Benzo, Fabian; Mendoza, Carolina; Queirolo, Marcelo; Sienra, Beatriz
CS Quimica Inorganica, Facultad de Quimica, Montevideo, Urug.
SO Polyhedron (1998), 17(13-14), 2295-2299
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
AB Nitrite ion competition has been measured for the base hydrolysis reaction of trans-Co(N-H3)4(NH2CH3)Xn+ ions (X = Cl-, Br-, NO3- and SO42-) in 1.0 M NaNO2 at 25°C. Both O- and N- bonded Co(NH3)4(NH2CH3)NO22+ are formed. Subsequently the Co(NH3)4(NH2CH3)ONO2+ isomer rearranges in OH- to give the thermodynamically more stable Co(NH3)4(NH2CH3)NO22+ ion. The total NO2- captured shows a slight dependence on the overall charge of the complex and on the nature of X (R = 2.2, 2.1, 3.6 and 1.2±0.5% for X = Cl-, Br-, NO3- and SO42-, resp.). These results differ from those observed with complexes of the type Co(NH3)5Xn+ and Co(NH2CH3)5Xn+ where X includes a variety of anions.
IT 210574-34-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(competition study for base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ complexes)
RN 210574-34-8 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κO]-, (OC-6-23)-(9CI) (CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1997:809063 CAPLUS
DN 128:146849
TI Infrared and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni
AU Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B.
CS Department of Physics, St. Gregorios College, Kottarakara, 691531, India
SO Journal of Solid State Chemistry (1997), 133(2), 407-415
CODEN: JSSCBI; ISSN: 0022-4596
PB Academic Press
DT Journal

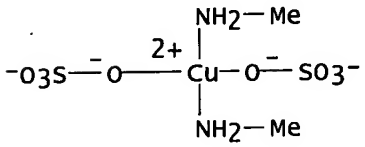
LA English

AB FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2·6H2O > (CH3NH3)2Ni (SO4)2·6H2O > (CH3NH3)2Zn(SO4)2·6H2O > Na2Cu(SO4)2·2H2O. The appearance of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and SO42- groups. The appearance of multiple bands in the bending and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mols. in (CH3NH3)2Cu(SO4)2·6H2O and (CH3NH3)2 Zn(SO4)2·6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2·6H2O.

IT 202406-44-8 202406-47-1 202406-49-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(IR and Raman spectra, internal vibrational mode assignments, and hydrogen bonding)

RN 202406-44-8 CAPLUS

CN Cuprate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, dihydrogen, hexahydrate (9CI) (CA INDEX NAME)

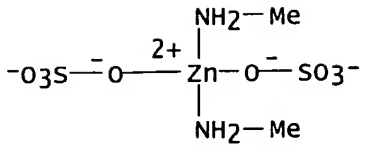


●2 H^+

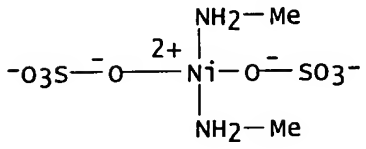
●6 H_2O

RN 202406-47-1 CAPLUS

CN Zincate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, dihydrogen, hexahydrate, (T-4)- (9CI) (CA INDEX NAME)



RN 202406-49-3 CAPLUS
CN Nickelate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, dihydrogen, hexahydrate (9CI) (CA INDEX NAME)



RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

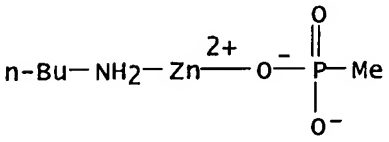
L10 ANSWER 14 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:704546 CAPLUS
DN 126:41873
TI Structure of Zn(O3PC2H4CO2H)·0.5C6H5NH2 and XANES-EXAFS study of the intercalation of amines into Zn(O3PR)·H2O zinc alkylphosphonates
AU Drumel, Stephanie; Janvier, Pascal; Bujoli-Doeuff, Martine; Bujoli, Bruno
CS IMN, UMR CNRS 110, Faculte des Sciences et des Techniques, Nantes, 44072, Fr.
SO Journal of Materials Chemistry (1996), 6(11), 1843-1847
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
AB From XANES-EXAFS expts., neither the dehydration nor the subsequent n-alkylamine intercalation in Zn(O3PCH3)·H2O appears to be topotactic. On the contrary, the whole process consists of breaking Zn-O bonds present in the hydrated material, so that no bridging oxygen remains in the inorg. sheet. This hypothesis is supported by the structural determination

of an aniline intercalate: Zn(O3PC2H4CO2H)·0.5C6H5NH2 [orthorhombic, space group Pbcn, a 29.880(6), b 8.526(2), c 14.720(3) Å, Z = 16, R = 0.043 and Rw = 0.047; 2063 observed reflections, I > 2σ(I)]. For steric reasons, only half of the zinc atoms are coordinated to aniline; the 2nd half of the metal atoms that are not bound to the amine retain the environment present in the initial anhydrous phase.

IT 184824-62-2
RL: PRP (Properties)
(XANES-EXAFS spectra of)

RN 184824-62-2 CAPLUS

CN Zinc, (1-butanamine)[methylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)



L10 ANSWER 15 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:652255 CAPLUS

DN 125:286037

TI Quantum-chemical studies on the mechanism of the novel reaction of oxidative amination of P4 in the copper(II) coordination sphere

AU Dorfman, Ya. A.; Abdreimova, R. R.

CS Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy of Sciences of Kazakhstan, Almaty, Kazakhstan

SO Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
CODEN: RJCCEY; ISSN: 1070-3284

PB MAIK Nauka/Interperiodica

DT Journal

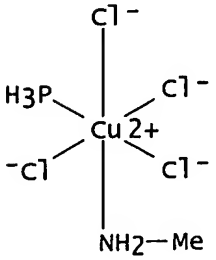
LA English

AB A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II)→Cu(0) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra- and interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions.

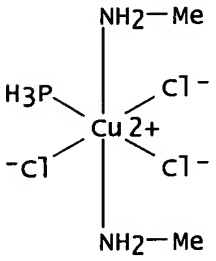
IT 182930-87-6 182930-88-7 182930-94-5

182930-97-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

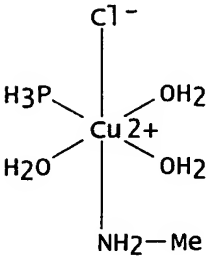
RN 182930-87-6 CAPLUS
CN Cuprate(2-), tetrachloro(methanamine)(phosphine)-, (OC-6-32)- (9CI) (CA INDEX NAME)



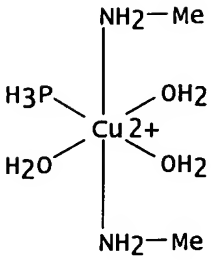
RN 182930-88-7 CAPLUS
CN Cuprate(1-), trichlorobis(methanamine)(phosphine)-, (OC-6-21)- (9CI) (CA INDEX NAME)



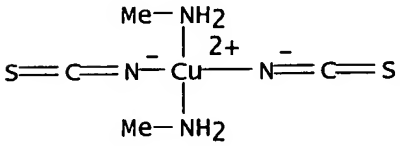
RN 182930-94-5 CAPLUS
CN Copper(1+), triaquachloro(methanamine)(phosphine)-, (OC-6-43)- (9CI) (CA INDEX NAME)



RN 182930-97-8 CAPLUS
CN Copper(2+), triaquabis(methanamine)(phosphine)-, (OC-6-22)- (9CI) (CA INDEX NAME)

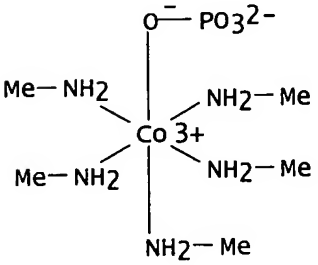


L10 ANSWER 16 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:130370 CAPLUS
DN 125:24833
TI Interaction of copper powder with nonaqueous solutions of methylammonium salts
AU Babich, O. A.; Kokozei, V. N.; Pavlenko, V. A.
CS Kiev. Gos. Univ., Kiev, Ukraine
SO Zhurnal Neorganicheskoi Khimii (1996), 41(1), 79-82
CODEN: ZNOKAQ; ISSN: 0044-457X
PB MAIK Nauka
DT Journal
LA Russian
AB The interaction of Cu powder with MeCN, MeOH, DMSO, and DMF solns. of methylammonium bromide, iodide, or thiocyanate was studied. Products of the interaction were isolated and identified. The crystalline structure of [Cu(CH3NH2)4]I2 was detd (monoclinic, P21/n, a = 7.088(1), b = 8.872(1), c = 10.590(1) Å, β = 95.29(1)°, V = 663.04 Å3, Z = 2, ρc = 2.212 g/cm3, μ(CuKα) = 390.3 cm-1, F(000) = 414, T = 20°, 1043 reflections with I > 3σ(I), R = 0.061, Rw = 0.090).
IT 57286-68-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from Cu and methylammonium salts in nonaq. solns.)
RN 57286-68-7 CAPLUS
CN Copper, bis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



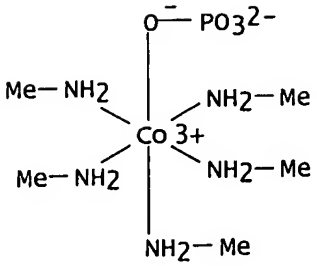
L10 ANSWER 17 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1996:10558 CAPLUS
DN 124:128031
TI Outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes. A temperature- and pressure-dependence kinetic study on the effects of the different {N5} groups
AU Martinez, Manuel; Pitarque, Mari-Angel
CS Facultat Quimica, Universitat Barcelona, Barcelona, E-08028, Spain
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (24), 4107-11
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry

DT Journal
LA English
AB Outer-sphere redox reactions between [Co{N5}(HnPO4)]n+[{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane (L)] and [Fe(CN)6]4- have been studied as a function of pH, {N5}, temperature and pressure. The effect of the size of the {N5} skeleton, has been investigated for the n = 0, 1, 2 systems in order to establish possible correlations between the size and charge of the cobalt(III) complex and the ion-pair formation constant, the electron-transfer rate constant, and the thermal and baric activation parameters. The values obtained indicate that the ion-pair formation consts. are the same, within exptl. error, for all the systems studied. The electron-transfer rate constant for a given degree (n = 1) of protonation of the [Co{N5}(HnPO4)]n+ complex increases on increasing the size of the monodentate amines, while an important decrease is observed when they are substituted by the N5 macrocycle (L) [2.6 + 10-3 s-1, {N5} = (NH3)5, 59 + 10-3 s-1, {N5} = (NH2Me)5, 0.73 + 10-3 s-1, {N5} = L; resp. at 35°C]. The activation enthalpies do not show any significant change, neither with decreasing charge on the cobalt complex nor with the size of the amine. The values of ΔS.thermod. and ΔV.thermod. vary considerably with the degree of protonation of the phosphate ligands and the size of the CoIII cavity of the complexes. The opposite trends observed for the values of ΔS.thermod. [8 J K-1 mol-1 for {N5} = (NH2Me)5 (n = 1); -61 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 32 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 17 cm3 mol-1 for {N5} = (NH3)5 (n = 0)] are related to the existence of an important increase in hydrogen bond formation in the cobalt(III) complex on going to the transition state.
IT 173178-22-8 173178-23-9
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes and temperature- and pressure-dependence kinetic effects of different {N5})
RN 173178-22-8 CAPLUS
CN Cobalt, pentakis(methanamine)[phosphato(3-)-O]-, conjugate monoacid, (OC-6-22)- (9CI) (CA INDEX NAME)

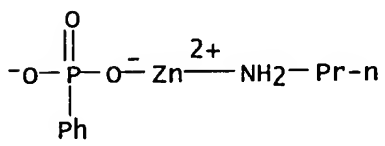


● H+

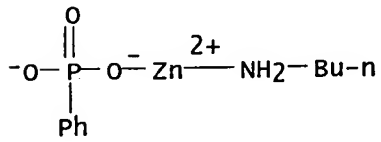
RN 173178-23-9 CAPLUS
CN Cobalt, pentakis(methanamine)[phosphato(3-)-O]-, (OC-6-22)- (9CI) (CA INDEX NAME)



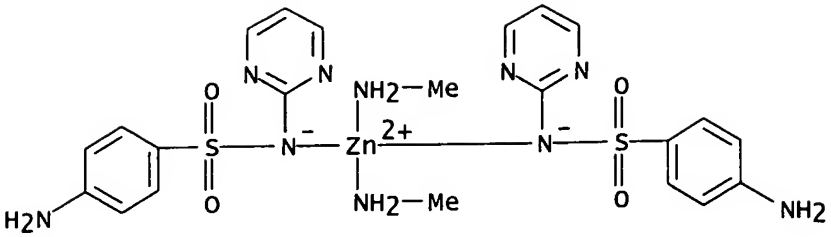
L10 ANSWER 18 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:899304 CAPLUS
DN 124:67877
TI Coordinative intercalation of alkylamines into layered zinc phenylphosphonate. Crystal structures from x-ray powder diffraction data
AU Poojary, Damodara M.; Clearfield, Abraham
CS Department of Chemistry, Texas AM University, College Station, TX, 77843, USA
SO Journal of the American Chemical Society (1995), 117(45), 11278-84
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Zn phenylphosphonate monohydrate takes up 1 mol of amine when contacted with liquid primary alkylamines. The mechanism of intercalation involves replacement of the coordinated H2O mol. by the amine mols. Although the composition of the intercalate Zn(O3PPh)(RNH2) is consistent with the anal. and spectroscopic data, there exist discrepancies in the observed interlayer d spacings of the intercalate with respect to that in the host compound The d spacing for the propylamine intercalate is in fact smaller than that in Zn phenylphosphonate itself. To understand this feature specifically and to explain the mechanism of amine intercalation in metal phosphonates in general, the authors determined the structures of the intercalates. The structures of Zn(O3PPh)(RNH2), R = -C3H9 (1), -C4H11 (2), -C5H13 (3), were solved ab initio from x-ray powder diffraction data and refined by Rietveld methods. All the compds. are isostructural, and they crystallize in the monoclinic space group P21/c with a 13.978(3), b 8.791(2), c 9.691(2) Å, and β 102.08(1)° for 1, a 14.698(4), b 8.957(3), c 9.712(3) Å, and β 102.465(3)° for 2, and a 16.267(3), b 8.935(2), c 9.695(2) Å, and β 102.32(1)° for 3. The structures of these intercalates are new and are different from that of the host compound although all of them are layered. In the intercalate the Zn atoms are tetrahedrally coordinated as opposed to octahedral coordination in the host compound.
IT 162050-25-1P 162050-26-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
RN 162050-25-1 CAPLUS
CN Zinc, [phenylphosphonato(2-)-O](1-propanamine)- (9CI) (CA INDEX NAME)



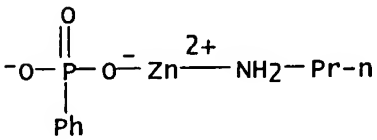
RN 162050-26-2 CAPLUS
CN Zinc, (1-butanamine)[phenylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)



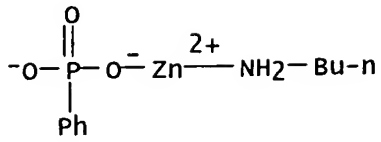
L10 ANSWER 19 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:676435 CAPLUS
DN 123:102111
TI Zinc sulfadiazines: novel topical antimicrobial agents for burns
AU Lee, A. R.; Huang, W. H.
CS Sch. Pharmacy, National Defense Med. Cent., Taipei, Taiwan
SO Journal of Pharmacy and Pharmacology (1995), 47(6), 503-9
CODEN: JPPMAB; ISSN: 0022-3573
PB Royal Pharmaceutical Society of Great Britain
DT Journal
LA English
AB Two new zinc sulfadiazine (Zn(SD)2)-amine complexes, zinc sulfadiazine-methylamine (Zn(SD)2(CH3NH2)2) and zinc sulfadiazine-ethylenediamine (Zn(SD)2(C2H8N2)3.H2O), were prepared and compared with silver sulfadiazine (AgSD). The compds. were readily obtained by reaction of zinc nitrate hexahydrate with sulfadiazine or its methylamine and ethylenediamine salts. Structure was established by X-ray crystallog. and UV-visible, IR and NMR spectroscopy. The products were effective, in-vitro, against Gram-pos. and Gram-neg. bacteria as well as fungus. However, their activity is partially reversed by p-aminobenzoic acid. Further investigations in burned mice revealed that these compds. displayed a potential value in the prevention and treatment of wound healing, and diminution of mortality and weight loss. The toxicity of Zn(SD)2 derivs. was much lower than that of AgSD. The better aqueous solubility and skin permeability may explain the reason for their superiority over AgSD in the efficacy for topical therapy. Zn(SD)2(CH3NH2)2 was consistently more potent and was chosen for further development in clin. uses. The similarity in complexation between Sn(SD)2(CH3NH2)2 and AgSD may be significant to distinguish that from any other Zn(SD)2 derivative in bioactivity.
IT 126830-36-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(zinc sulfadiazines and novel topical antimicrobial agents for burns)
RN 126830-36-2 CAPLUS
CN Zinc, bis(4-amino-N-2-pyrimidinylbenzenesulfonamidato)bis(methanamine)-, (T-4)- (9CI) (CA INDEX NAME)



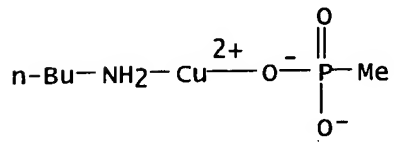
L10 ANSWER 20 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1995:419353 CAPLUS
DN 122:229146
TI Intercalation of alkylamines into dehydrated and hydrated zinc phenylphosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Department of Chemistry, Texas A and M Univ., College Station, TX, 77843, USA
SO Journal of Materials Chemistry (1995), 5(2), 315-18
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
AB Primary amines, CnH2n+1NH2 (n = 3-8), were intercalated into layered anhydrous Zn phenylphosphonate Zn(O3PPh) and its monohydrate Zn(O3PPh).H2O when the host compds. were brought into contact with liquid amines. In both cases, 1 mol of amine was intercalated forming layered compds. Zn(O3PPh).(RNH2) as characterized by powder x-ray diffraction, TG and IR spectroscopy. The amines coordinate to the Zn atoms at the site vacated by the H2O mol. A plot of the interlayer distances of the intercalates vs. the number of C atoms in the alkyl chain of the amine gives a straight line with a slope of 1.24 Å, which indicates that the alkyl chains are most likely packed as an interdigitated monolayer with a tilt angle of 78° with respect to the mean plane of the layer. A comparison of the intercalation reactions of Zn, Co and Cu Me- and phenyl-phosphonates is included in the discussion section.
IT 162050-25-1P 162050-26-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 162050-25-1 CAPLUS
CN Zinc, [phenylphosphonato(2-)-O](1-propanamine)- (9CI) (CA INDEX NAME)



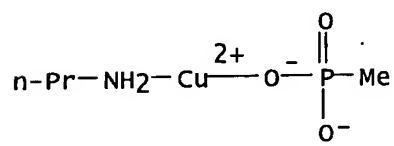
RN 162050-26-2 CAPLUS
CN Zinc, (1-butanamine)[phenylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)



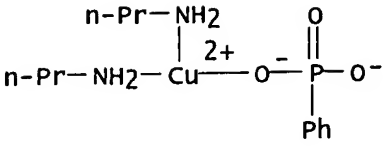
L10 ANSWER 21 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1993:234154 CAPLUS
DN 118:234154
TI Intercalation of alkylamines into layered copper phosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Chemistry of Materials (1993), 5(4), 495-9
CODEN: CMATEX; ISSN: 0897-4756
DT Journal
LA English
AB Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3)·(RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates.
IT 141848-52-4P 147578-74-3P 147578-79-8P
147578-80-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer distances of)
RN 141848-52-4 CAPLUS
CN Copper, (1-butanamine)[methylphosphonato(2-)-O]- (9CI) (CA INDEX NAME)



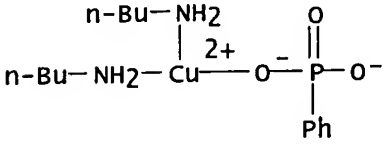
RN 147578-74-3 CAPLUS
CN Copper, [methylphosphonato(2-)-O](1-propanamine)- (9CI) (CA INDEX NAME)



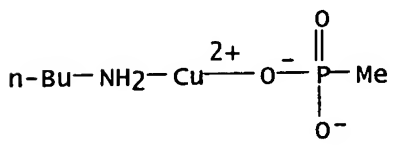
RN 147578-79-8 CAPLUS
CN Copper, [phenylphosphonato(2-)-O]bis(1-propanamine)- (9CI) (CA INDEX NAME)



RN 147578-80-1 CAPLUS
CN Copper, bis(1-butanamine)[phenylphosphonato-O]- (9CI) (CA INDEX NAME)



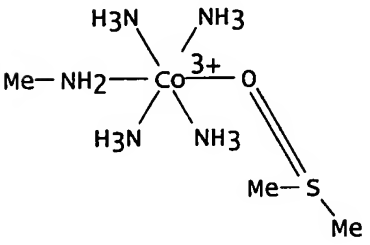
L10 ANSWER 22 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1992:419105 CAPLUS
DN 117:19105
TI Synthesis, crystal structures, and coordination intercalation behavior of two copper phosphonates
AU Zhang, Yiping; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Inorganic Chemistry (1992), 31(13), 2821-6
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
AB Cu(O3PMe).H2O and Cu(O3PPh).H2O were synthesized and their structures determined Cu(O3PMe).H2O is monoclinic: space group P21/c, a 8.495(4), b 7.580(4), c 7.289(4) Å, β 90.08 (4)°, Z = 4, R = 0.030, Rw = 0.041. The structure is layered as formed by unusual 5-coordinate distorted tetragonal pyramidal Cu atoms. One O of each phosphonate bonds to 2 Cu atoms forming a chain, while the other 2 phosphonate O atoms bond to 2 Cu atoms in an adjacent chain. The base of the pyramid consists of 3 phosphonate O atoms and the coordinated H2O mol. All H bonds are of the intralayer type, so only van der Waals forces exist between adjacent layers. Amines are coordinatively intercalated with layer expansion. Cu(O3PPh).H2O is orthorhombic: space group Pbca, a 7.5547(4), b 7.4478(6), c 27.928(1) Å, Z = 8, R = 0.037 and Rw = 0.043. The coordination about the Cu atoms and the layer structure are identical to those of the O3PMe compound The Ph rings in the interlamellar space are oriented at a 98° angle to each other in adjacent rows. These structures are compared to those of other layered divalent phosphonates and Cu phosphites.
IT 141848-52-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer spacing of intercalation compound)
RN 141848-52-4 CAPLUS
CN Copper, (1-butanamine)[methylphosphonato(2-)-O]- (9CI) (CA INDEX NAME)



L10 ANSWER 23 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1992:50338 CAPLUS
DN 116:50338
TI Synthesis and characterization of trans-[Co(NH3)4(NH2CH3)L]3+ [L = (CH3)2SO or (CH3)2NCHO] complexes
AU Sienra, Beatriz; Massaferro, Adriana
CS Fac. Quim., Montevideo, Urug.
SO Polyhedron (1991), 10(17), 2075-8
CODEN: PLYHDE; ISSN: 0277-5387
DT Journal
LA English
AB trans-[Co(NH3)4(NH2Me)Me2SO]X3 (X = ClO4, Br) and trans-[Co(NH3)4(NH2Me)Me2NCHO](ClO4)3 are prepared by Ag+-induced solvolysis of trans-[Co(NH3)4(NH2Me)X]2+ (X = Cl or Br) complexes in DMSO or DMF. The complexes were characterized by electronic, IR and 1H NMR. DMSO and DMF are bonded through the oxygen atom. The trans-complexes obtained are not contaminated with the cis-isomers.
IT 138521-44-5P 138521-45-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 138521-44-5 CAPLUS
CN Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-O]-, (OC-6-23)-, triperchlorate (9CI) (CA INDEX NAME)

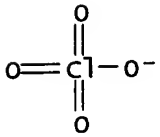
CM 1

CRN 138521-43-4
CMF C3 H23 Co N5 O S
CCI CCS

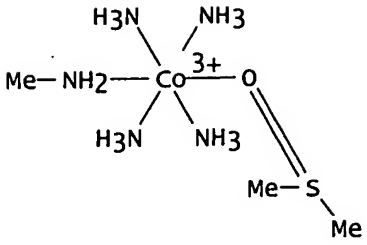


CM 2

CRN 14797-73-0
CMF Cl O4



RN 138521-45-6 CAPLUS
CN Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-O]-, tribromide, (OC-6-23)- (9CI) (CA INDEX NAME)

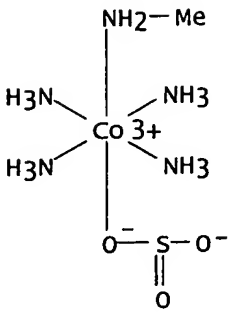


● 3 Br^-

L10 ANSWER 24 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1991:258445 CAPLUS
DN 114:258445
TI Synthesis, characterization and some reactions of trans-tetraamminebromo(methanamine)cobalt(2+) and trans-tetraammine(methanamine(nitratocobalt(2+) complexes
AU Sienra, B.; Massaferro, A.; Piriz Mac-Coll, C. R.
CS Univ. Republica, Montevideo, Urug.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1990), 590, 222-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
AB The preparation of trans-[Co(NH3)4(CH3NH2)Br]2+ (I) and trans-[Co(NH3)4(CH3NH2)(NO3)]2+ is described. The UV-visible spectra of the complexes indicate a decrease of the ligand field compared to the parent pentaammines. IR spectra match with the pattern of the corresponding pentaammines. The catalyzed (by Hg2+) aquation of I occurred with retention of the stereochem. configuration. The base hydrolysis (studied at 25°) products show trans to cis rearrangement for both complexes. 1H NMR spectroscopy is used for identification of the stereochem. configuration of the compds.
IT 134066-33-4P, trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of, in presence of nitric acid)
RN 134066-33-4 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-O]-, (OC-6-23)-, nitrate (9CI) (CA INDEX NAME)

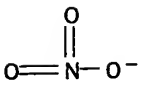
CM 1

CRN 134066-32-3
CMF C H17 Co N5 O3 S
CCI CCS

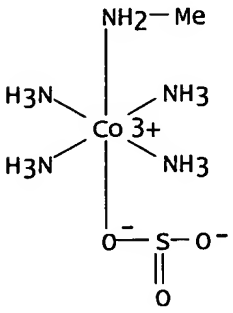


CM 2

CRN 14797-55-8
CMF N O3



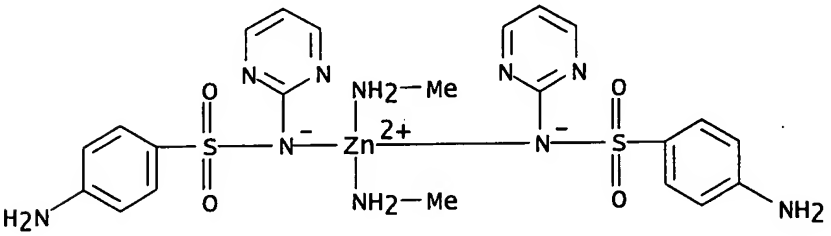
IT 134066-26-5P, trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrogen bromide)
RN 134066-26-5 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-O]-, bromide, (OC-6-23)-(9CI) (CA INDEX NAME)



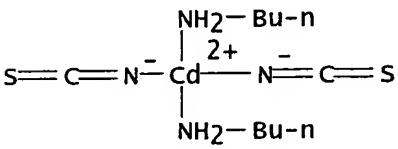
● Br⁻

L10 ANSWER 25 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1990:209715 CAPLUS
DN 112:209715
TI A facile synthesis of zinc sulfadiazine derivatives
AU Lee, An Rong; Huang, Wen Hsin; Lai, Jin Shing; Chan, Shu Fei
CS Sch. Pharm., Natl. Def. Med. Cent., Taipei, Taiwan

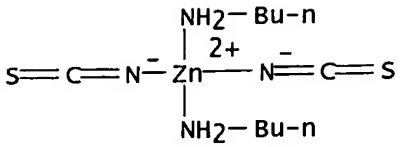
SO Zhonghua Yaoxue Zazhi (1989), 41(4), 345-8
CODEN: CYHCEX; ISSN: 1016-1015
DT Journal
LA English
AB Treatment of sulfadiazine with Zn(NO3)2 in the presence of NH4OH, MeNH2, or H2NCH2CH2NH2 gave the corresponding title complexes, whose mol. structures were determined
IT 126830-36-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
RN 126830-36-2 CAPLUS
CN Zinc, bis(4-amino-N-2-pyrimidinylbenzenesulfonamidato)bis(methanamine)-, (T-4)- (9CI) (CA INDEX NAME)



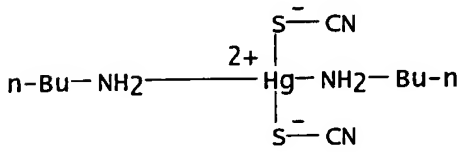
L10 ANSWER 26 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1987:584014 CAPLUS
DN 107:184014
TI Study of the bond strength in complex compounds by proton NMR
AU Galitskaya, S. M.; Pavlenko, L. I.
CS USSR
SO Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
CODEN: VLPIAZ; ISSN: 0460-0436
DT Journal
LA Russian
AB Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN, NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases in the order CN > NCS # NCSe.
IT 38255-54-8 110945-33-0 110946-24-2
RL: PRP (Properties)
(bond energy in, NMR in study of)
RN 38255-54-8 CAPLUS
CN Cadmium, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)



RN 110945-33-0 CAPLUS
CN Zinc, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)



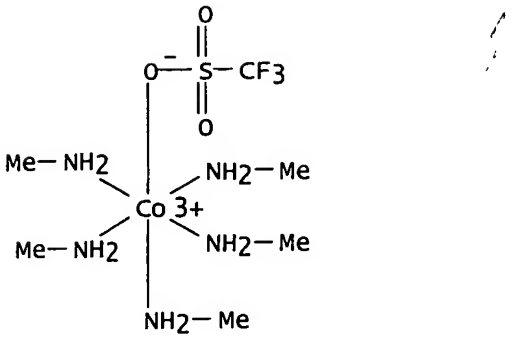
RN 110946-24-2 CAPLUS
CN Mercury, bis(1-butanamine-N)bis(thiocyanato-S)-, (T-4)- (9CI) (CA INDEX NAME)



L10 ANSWER 27 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1986:507276 CAPLUS
DN 105:107276
TI Pentakis(methanamine)(trifluoromethanesulfonato-O) complexes of chromium(III), cobalt(III), and rhodium(III)
AU Lawrance, Geoffrey A.; Sargeson, Alan M.
CS Dep. Chem., Univ. Newcastle, 2308, Australia
SO Inorganic Syntheses (1986), 24, 279-82
CODEN: INSYA3; ISSN: 0073-8077
DT Journal
LA English
AB [M(NH2Me)5(OSO2CF3)](SO3CF3)2 (M = Co, Cr, Rh) were prepared from [M(NH2Me)5Cl]Cl2 and CF3SO3H.
IT 90065-88-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from cobalt chloro methylamine complex and trifluoromethanesulfonic acid)
RN 90065-88-6 CAPLUS
CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

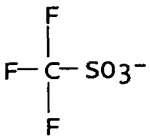
CM 1

CRN 84254-64-8
CMF C6 H25 Co F3 N5 O3 S
CCI CCS



CM 2

CRN 37181-39-8
CMF C F3 O3 S



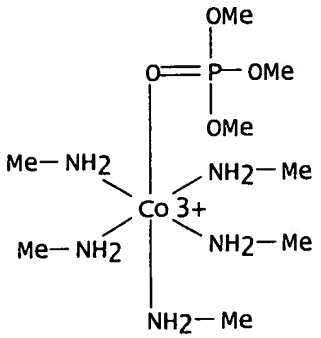
L10 ANSWER 28 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1986:141030 CAPLUS
DN 104:141030
TI Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile
AU Curtis, Neville J.; Lawrance, Geoffrey A.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
AB Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. ΔS.thermod. and ΔV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis(methylamine) complexes. These results parallel earlier observations of ΔS.thermod. and ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed.
IT 100681-45-6P 100681-49-0P 100681-50-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and kinetics of acid aquation of)

RN 100681-45-6 CAPLUS
CN Cobalt(3+), pentakis(methanamine)(trimethyl phosphate-O''')-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)

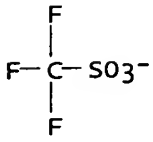
CM 1

CRN 100681-44-5
CMF C8 H34 Co N5 O4 P
CCI CCS



CM 2

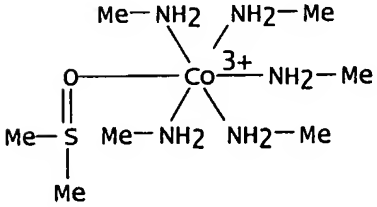
CRN 37181-39-8
CMF C F3 O3 S



RN 100681-49-0 CAPLUS
CN Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-O]-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)

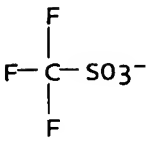
CM 1

CRN 100681-48-9
CMF C7 H31 Co N5 O S
CCI CCS



CM 2

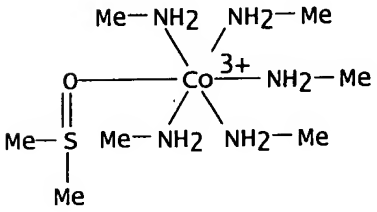
CRN 37181-39-8
CMF C F3 O3 S



RN 100681-50-3 CAPLUS
CN Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-O]-, (OC-6-22)-, triperchlorate (9CI) (CA INDEX NAME)

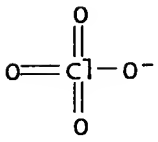
CM 1

CRN 100681-48-9
CMF C7 H31 Co N5 O S
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4

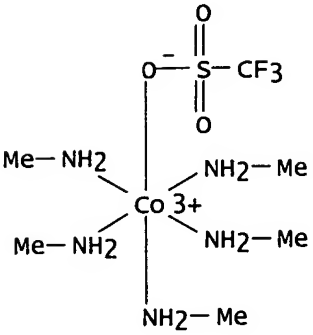


IT 90065-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reactions of, with neutral ligands)
RN 90065-88-6 CAPLUS
CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

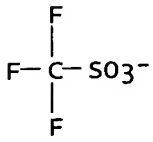
CRN 84254-64-8
CMF C6 H25 Co F3 N5 O3 S

CCI CCS

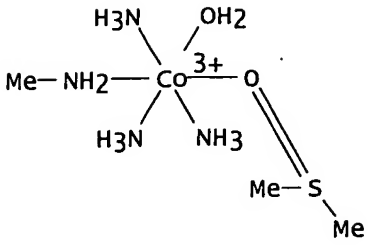


CM 2

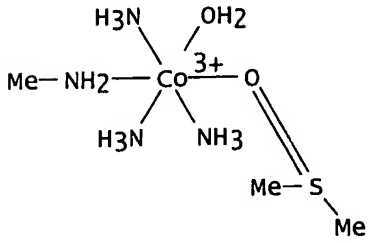
CRN 37181-39-8
CMF C F3 O3 S



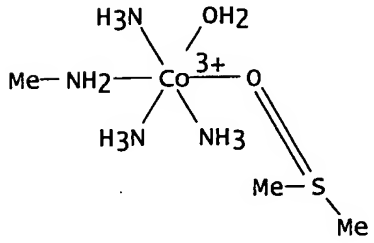
L10 ANSWER 29 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1986:121904 CAPLUS
DN 104:121904
TI Formation and transformation of amminecarbonatocobalt(III) complexes
AU Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R.
CS Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
AB [CoCO3(NH3)5]Cl04.H2O, trans-[CoCO3(NH3)4(15NH3)]Cl04, and trans-[CoCO3(NH3)4(NH2Me)]Cl04 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. The products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific.
IT 100788-52-1P 100838-96-8P 100838-97-9P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from carbonato complex in acidified DMSO)
RN 100788-52-1 CAPLUS
CN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-O]-, (OC-6-44)- (9CI) (CA INDEX NAME)



RN 100838-96-8 CAPLUS
CN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-O]-, (OC-6-43)- (9CI) (CA INDEX NAME)



RN 100838-97-9 CAPLUS
CN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-O]-, (OC-6-34)- (9CI) (CA INDEX NAME)



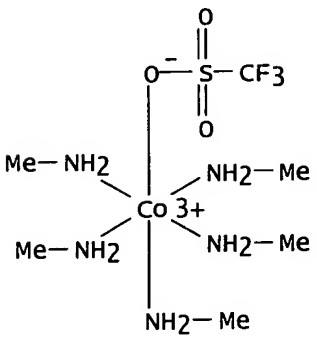
L10 ANSWER 30 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1986:96513 CAPLUS
DN 104:96513
TI Hydrolysis of coordinated trifluoromethanesulfonate from cobalt(III), rhodium(III), iridium(III) and chromium(III) pentaamines
AU Curtis, Neville J.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan M.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(4), 484-8
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
AB Base hydrolysis and aquation of M(NH3)5(OSO2CF3)2+ (M = Co, Rh, Ir, Cr) and M(NH2CH3)5(OSO2CF3)2+ (M = Co, Rh, Cr) complexes at 25° and ionic strength 1.0 M are reported. The N-methylation of the ammine ligand causes a marked enhancement of the rate of base hydrolysis reactions with kMe/kH of 2100 (Co), 150 (Rh), and 800 (Cr). only minor enhancements

occur for aquation with Co and Rh, while there is a minor rate diminution with Cr. Pos. activation entropies for base hydrolysis of M(NH3)5(OSO2CF3)2+ (M = Co, Ir) and competition expts. with azide ion in basic solution as well as the absence of the competing ion in the rate law allow a dissociative conjugate-base mechanism for all complexes. The variation in rate enhancement from ammine to methylamine compds. and the competition studies in base with azide ion chiefly reflect differences in steric interactions due to differing metal-ligand bond lengths rather than any mechanistic diversity. Variations in competition behavior for RhIII), Cr(III), and Co(III) appear to reflect relative lifetimes of the intermediate of reduced coordination number The variations in aquation are much smaller and do not allow any certainty in mechanistic assertions. Marked accelerations of rates for both acid and base hydrolyses (.apprx.103-106-fold) occur consistently for all trifluoromethanesulfonato complexes compared with those of halo of analogs.

IT 84254-64-8
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, kinetics of)

RN 84254-64-8 CAPLUS

CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)- (9CI) (CA INDEX NAME)



L10 ANSWER 31 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:521855 CAPLUS

DN 101:121855

TI Synthetically versatile (trifluoromethanesulfonato)metal amine complexes

AU Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan M.

CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia

SO Inorganic Chemistry (1984), 23(19), 2940-7
CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

AB Facile preparation routes to complexes of the labile unidentate coordinated -OSO2CF3 ion are reported for M(NH3)5(OSO2CF3)n+ (M = Rh, Ir, Cr, Ru, n = 2, M = Pt, n = 3), M(NH2Me)5(OSO2CF3)2+ (M = Co, Rh, Cr), cis-M(en)2(OSO2CF3)2+ (M = Rh, Ir, Cr, and trans-M(en)2Cl(OSO2CF3)+ (M = Rh, Ir). The utility of these synthetically versatile intermediates in the preparation of a variety of complexes containing neutral ligands is illustrated. Rate consts. for the aquation of the triflato complexes in 0.1M CF3SO3H at 25° span 3 orders of magnitude and for the pentaammine complexes show a reactivity order of Ru > Co .apprx. Cr .apprx. Rh » Ir > Pt. For the pentakis(methylamine) complexes, the aquation rate is greater for Co, slightly greater for Rh, and smaller for

Cr in comparison to the corresponding pentaammine complexes. The aquations of M(en)2X(OSO2CF3)+ proceed largely without isomerization (<5%), and the triflato complexes are prepared stereospecifically by this route. For the cis-M(en)2(OSO2CF3)2+ ions, consecutive 1st-order aquation processes are observed with rate consts. k1 .apprx. 2k2.

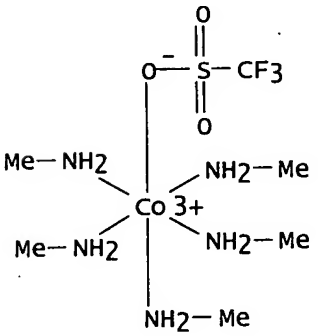
IT 90065-88-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of aquation of)

RN 90065-88-6 CAPLUS

CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

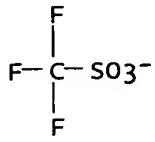
CM 1

CRN 84254-64-8
CMF C6 H25 Co F3 N5 O3 S
CCI CCS



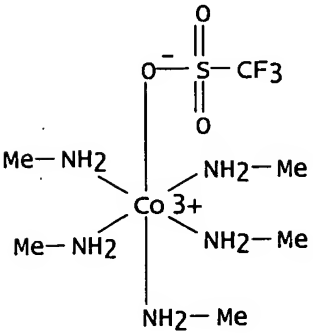
CM 2

CRN 37181-39-8
CMF C F3 O3 S

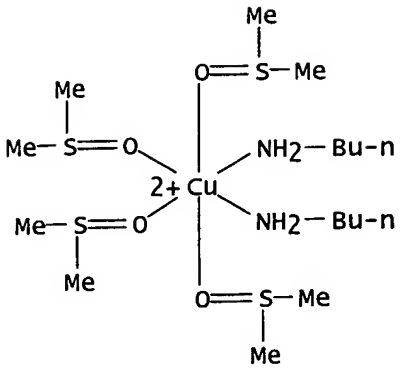


L10 ANSWER 32 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1983:100163 CAPLUS
DN 98:100163
TI (Trifluoromethanesulfonato-O)pentaammine complexes: versatile synthetic intermediates
AU Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan M.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia
SO Inorganic Chemistry (1983), 22(5), 846-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal

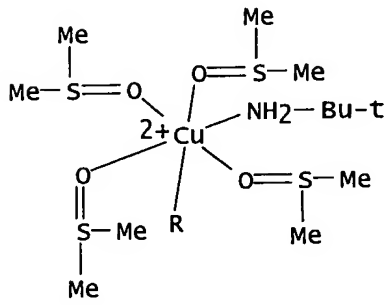
LA English
AB [M(NH3)5(OSO2CF3)](CF3SO3)n, where M = Cr(III), Rh(III), Ir(III), Ru(III), and Pt(IV), were prepared in essentially quant. yields from the reactions of [M(NH3)5Cl]Cln in CF3SO3H. The rate consts. for aquation of [M(NH3)5(OSO2CF3)](CF3SO3)n at 25° (0.1M CF3SO3H) indicate a reactivity order of Ru(III) > Rh(III) > Cr(III) > Pt(IV) > Ir(III). Aquation rate consts. for the [M(NH2Me)5(OSO2CF3)]2+ ions (M = Co(III), Rh(III), Cr(III)) were determined, and k(NH2Me)/k(NH3) ratios are 4.2, 1.7, and 0.051 for the Co(III), Rh(III), and Cr(III) complexes, resp.
IT 84254-64-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(aquation of, kinetics of)
RN 84254-64-8 CAPLUS
CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)- (9CI) (CA INDEX NAME)

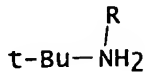


L10 ANSWER 33 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1980:153821 CAPLUS
DN 92:153821
TI Complexing of copper(II) salts with pyridines and primary aliphatic amines in dimethyl sulfoxide
AU Dulova, V. I.; Brezhe, A. L.; Molchanova, N. R.; Artyukhova, E. P.
CS Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SO Koordinatsionnaya Khimiya (1980), 6(2), 248-51
CODEN: KOKHDC; ISSN: 0132-344X
DT Journal
LA Russian
AB Instability consts. were determined spectrophotometrically and heats of coordination were determined calorimetrically for 1:1 and 1:2 complexes by assuming equilibrium of the type Cu(DMSO)62+ + 2L .dblharw. Cu(DMSO)5L2+ + DMSO; Cu(DMSO)5L2+ + L .dblharw. Cu(DMSO)4L22+ + DMSO. The relative importance of bonding in these complexes is discussed.
IT 73358-71-1P 73358-73-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in DMSO)
RN 73358-71-1 CAPLUS
CN Copper(2+), bis(1-butanamine)tetrakis[sulfinylbis[methane]-O]- (9CI) (CA INDEX NAME)



RN 73358-73-3 CAPLUS
CN Copper(2+), bis(2-methyl-2-propanamine)tetrakis[sulfinylbis[methane]-O]-(9CI) (CA INDEX NAME)



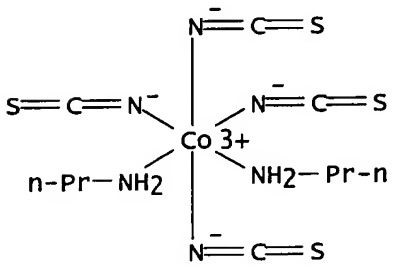


L10 ANSWER 34 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1978:452589 CAPLUS
DN 89:52589
TI New tetrathiocyanatodiaminechromates with aliphatic monoamines
AU Ganescu, I.; Varhelyi, C.; Futo, F.; Brinzan, G.
CS Chem. Fak., Univ. Craiova, Craiova, Rom.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1978), 439, 282-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA German
AB [Cr(NCS)4L2]- (L = PrNH2, BuNH2) were prepared by a substitution reaction of K3[Cr(NCS)6] with L in the molten state. Twenty complex salts of the type R.H[Cr(NCS)4L2] (L = amine) and 20 Co-amine complexes with [Co(NCS)4L2]- were isolated. The complexes were characterized by IR and UV spectra.
IT 67008-64-4P 67008-65-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 67008-64-4 CAPLUS
CN Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-

propanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 66915-22-8
CMF C10 H18 Co N6 S4
CCI CCS



CM 2

CRN 30649-39-9
CMF C18 H36 Co N4 O2
CCI CCS

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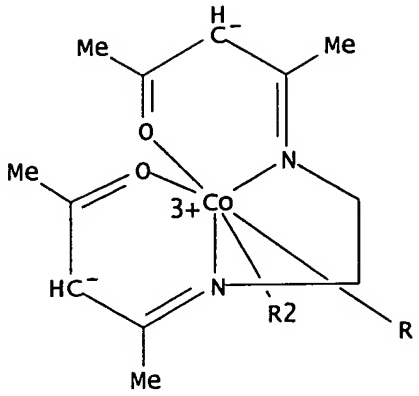

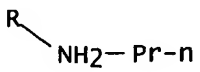

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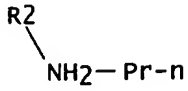
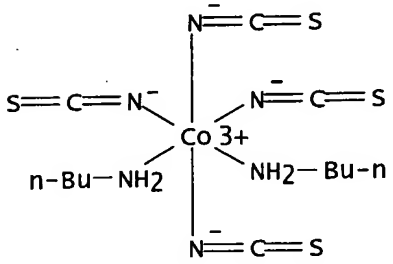


RN 67008-65-5 CAPLUS

CN Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-butanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)

CM 1

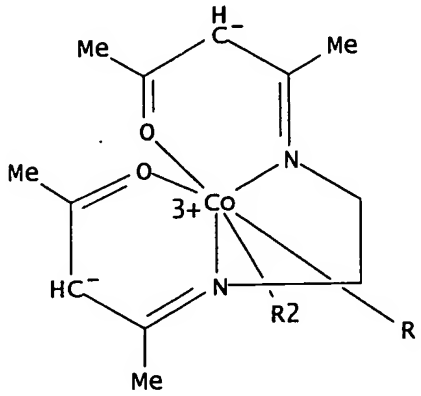
CRN 66915-23-9
CMF C12 H22 Co N6 S4
CCI CCS

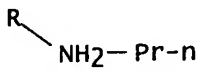


CM 2

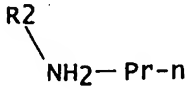
CRN 30649-39-9
CMF C18 H36 Co N4 O2
CCI CCS

PAGE 1-A





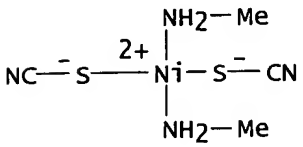
PAGE 2-A



L10 ANSWER 35 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1977:83070 CAPLUS
DN 86:83070
TI Heterogeneous reactions of solid nickel(II) complexes. X. Study of stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
AB Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.
IT 61896-84-2P 61896-86-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
RN 61896-84-2 CAPLUS
CN Nickel, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

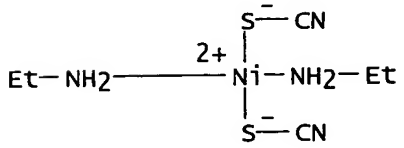
CRN 61896-83-1
CMF C4 H10 N4 Ni S2
CCI CCS



RN 61896-86-4 CAPLUS
CN Nickel, bis(ethanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 61896-85-3
CMF C6 H14 N4 Ni S2
CCI CCS



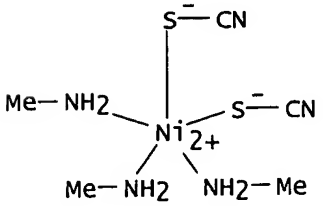
IT 61896-80-8P 61896-82-0P

RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)

RN 61896-80-8 CAPLUS
CN Nickel, tris(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

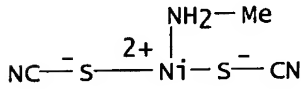
CRN 61896-79-5
CMF C5 H15 N5 Ni S2
CCI CCS



RN 61896-82-0 CAPLUS
CN Nickel, (methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

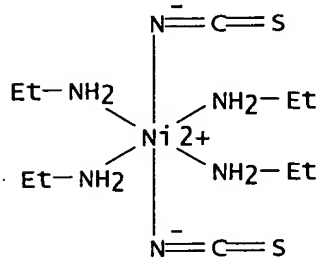
CM 1

CRN 61896-81-9
CMF C3 H5 N3 Ni S2
CCI CCS



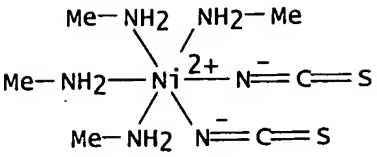
IT 61876-10-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

RN 61876-10-6 CAPLUS
CN Nickel, tetrakis(ethanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA INDEX NAME)

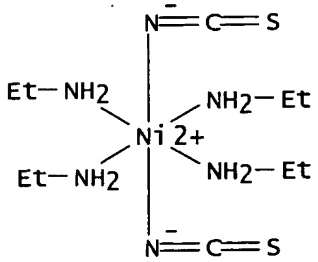


RN 61914-81-6 CAPLUS
CN Nickel, tetrakis(methanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA

INDEX NAME)



L10 ANSWER 36 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1977:83011 CAPLUS
DN 86:83011
TI Isomerism of nickel(II) complexes. VIII. Study of isomerism of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
AB Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2Me)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the monomer isomerizes to the green pseudooctahedral polymer. Steric effects in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic spectra.
IT 61876-10-6P 61896-84-2P 61896-86-4P
61914-81-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61876-10-6 CAPLUS
CN Nickel, tetrakis(ethanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA INDEX NAME)

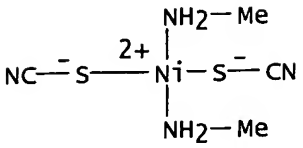


RN 61896-84-2 CAPLUS
CN Nickel, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 61896-83-1
CMF C4 H10 N4 Ni S2

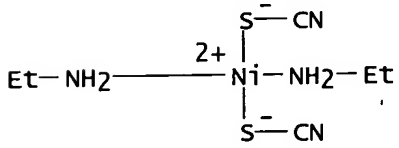
CCI CCS



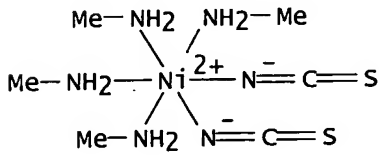
RN 61896-86-4 CAPLUS
CN Nickel, bis(ethanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 61896-85-3
CMF C6 H14 N4 Ni S2
CCI CCS



RN 61914-81-6 CAPLUS
CN Nickel, tetrakis(methanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA INDEX NAME)



L10 ANSWER 37 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1976:571027 CAPLUS
DN 85:171027
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.
CS Kiev. Gos. Univ., Kiev, USSR
SO Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg. Khim., Novosibirsk, USSR.
CODEN: 34BFAN
DT Conference
LA Russian
AB Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the

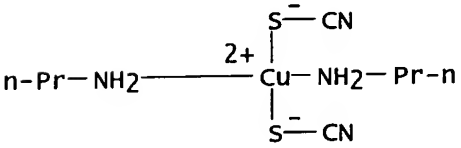
XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment.

IT 60865-90-9P 60865-92-1P 60865-94-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 60865-90-9 CAPLUS
CN Copper, bis(1-propanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

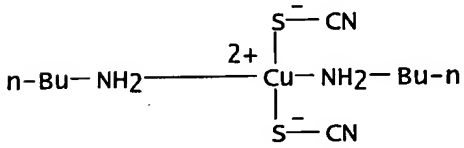
CRN 60865-89-6
CMF C8 H18 Cu N4 S2
CCI CCS



RN 60865-92-1 CAPLUS
CN Copper, bis(1-butanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

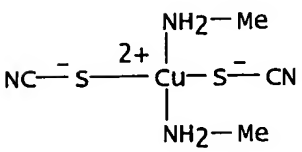
CRN 60865-91-0
CMF C10 H22 Cu N4 S2
CCI CCS



RN 60865-94-3 CAPLUS
CN Copper, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 60865-93-2
CMF C4 H10 Cu N4 S2
CCI CCS



L10 ANSWER 38 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1976:425322 CAPLUS
DN 85:25322
TI The cobaltous amine reaction. II. Cobalt complexes of barbiturates, methimazole, methylthiouracil, naphazoline, phenytoin, sulfathiazole and theophylline
AU Bult, A.
CS Lab. Pharm. Anal. Chem., State Univ. Groningen, Groningen, Neth.
SO Pharmaceutisch Weekblad (1976), 111(17), 385-93
CODEN: PHWEAW; ISSN: 0031-6911
DT Journal
LA English
AB The complexes of the composition CoX2(amine)2(X = anion of barbital, hexobarbital, methylphenobarbital, pentobarbital, phenobarbital, theophylline, and sulfathiazole; amine = isobutylamine, isopropylamine or NH3) are pseudo tetrahedral (Co(II) complexes. Co(II) coordinates with the barbiturates via N-I, with theophylline via N-7 or N-9, with sulfathiazole via the tertiary N atom of the thiazole ring. With X = anion of phenytoin the octahedral complex Co(II)X2(amine)4 is formed. This pink complex dissolves CHCl3 to a violet tetrahedral complex. With a large excess of amine the tetrahedral is converted to an octahedral. The donor atom in X is N-3. With X = naphazoline the (pseudo) tetrahedral Co(II) complexes CoX2(acetate)2 and [CoX4](ClO4)2 are prepared The pos. charge of Co2+ is compensated by acetate (coordinated) and ClO4- (uncoordinated resp. The donor atom in X is the tertiary Atom. With use of the ir spectra of previously described Co(II) complexes of methimazole a contribution to the interpretation of the ir spectrum of this drug is given. With X = anion of methylthiouracil some Co(III) complexes with the average composition CoX2(amine)n (n = .apprx.3) are prepared The available data
are insufficient for assigning the structure.
IT 59710-34-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
RN 59710-34-8 CAPLUS
CN Cobalt, bis(4-amino-N-2-thiazolylbenzenesulfonamidato-NN)bis(2-methyl-1-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

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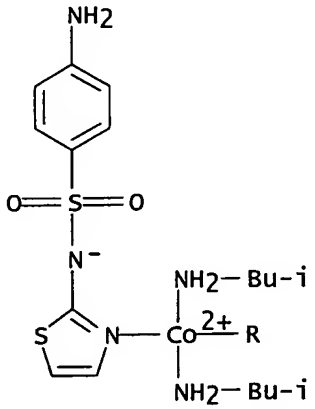

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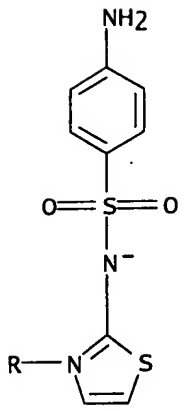
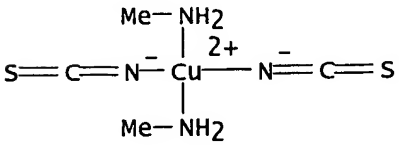
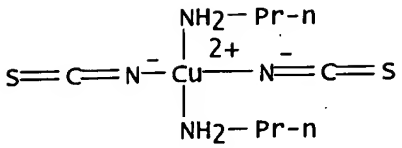


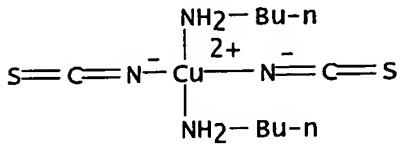
L10 ANSWER 39 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1975:587668 CAPLUS
DN 83:187668
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
AB Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2, RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded. The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are N-bonded.
IT 57286-68-7P 57286-70-1P 57286-71-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 57286-68-7 CAPLUS
CN Copper, bis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



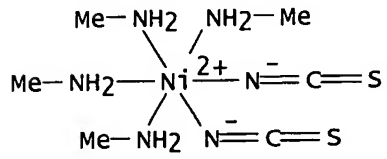
RN 57286-70-1 CAPLUS
CN Copper, bis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



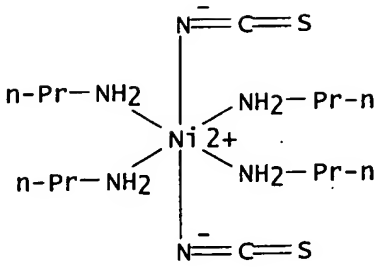
RN 57286-71-2 CAPLUS
CN Copper, bis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



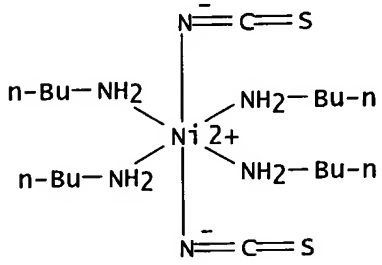
L10 ANSWER 40 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1975:38050 CAPLUS
DN 82:38050
TI Nickel aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
AB Amines in MeOH were added to MeOH solns. containing KSCN or KSeCN and Ni(NO3)2.6-H2O to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined
IT 54438-97-0P 54438-99-2P 54439-01-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54438-97-0 CAPLUS
CN Nickel, tetrakis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



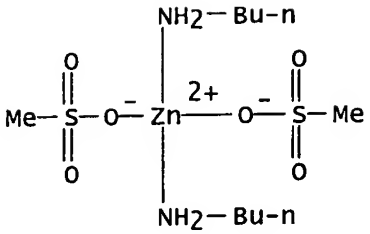
RN 54438-99-2 CAPLUS
CN Nickel, tetrakis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



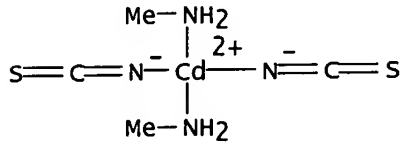
RN 54439-01-9 CAPLUS
CN Nickel, tetrakis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)



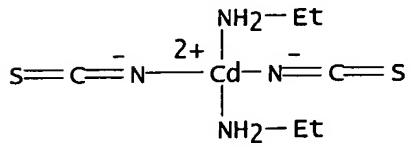
L10 ANSWER 41 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1974:530234 CAPLUS
DN 81:130234
TI Chemistry of substituted sulfuric acids. VIII. Methanesulfonates of tin(II), tin(IV), and zinc(II)
AU Paul, Ram C.; Kapila, V. P.; Sharma, S. K.
CS Dep. Chem., Panjab Univ., Chandigarh, India
SO Indian Journal of Chemistry (1974), 12(6), 651-2
CODEN: IJOCAP; ISSN: 0019-5103
DT Journal
LA English
AB SnCl2(MeSO3)2, Sn(MeSO3)2, and Zn(MeSO3)2 were prepared by reacting the resp. metal chlorides with MeSO3H. Their 1:2 adducts with pyridine and BuNH2 were prepared and their conductances studied in MeSO3H. The presence of phases Cs2M(MeSO3)4 (M = Sn or Zn) was indicated by f.p. detns. of the M(MeSO3)2-CsMeSO3 systems.
IT 53396-13-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53396-13-7 CAPLUS
CN Zinc, bis(1-butanamine)bis(methanesulfonato-O)-, (T-4)- (9CI) (CA INDEX NAME)



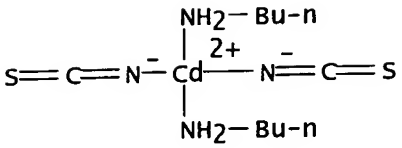
L10 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1972:520272 CAPLUS
DN 77:120272
TI Cadmium aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Galitskaya, S. M.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
AB The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu, do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to the Cd atom via the N atom.
IT 38255-49-1 38255-51-5 38255-54-8
38441-98-4
RL: PRP (Properties)
(ir spectrum of, structure in relation to)
RN 38255-49-1 CAPLUS
CN Cadmium, bis(methanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)



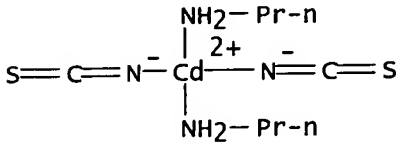
RN 38255-51-5 CAPLUS
CN Cadmium, bis(ethanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)



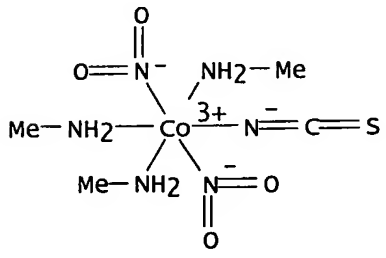
RN 38255-54-8 CAPLUS
CN Cadmium, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)



RN 38441-98-4 CAPLUS
CN Cadmium, bis(1-propanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)

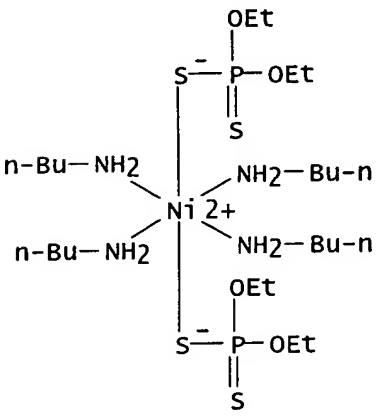


L10 ANSWER 43 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1972:442560 CAPLUS
DN 77:42560
TI Nitro methylamine complexes of cobalt(III)
AU Ganiev, A. G.; Tukhtaev, Sh. Sh.; Ikramov, Kh. U.
CS Inst. Yad. Fiz., Kiev, USSR
SO Zhurnal Neorganicheskoi Khimii (1972), 17(5), 1384-7
CODEN: ZNOKAQ; ISSN: 0044-457X
DT Journal
LA Russian
AB MeNH2 reacts with [Co(NO2)6]3- to give mixed complexes. K[Co(MeNH2)2(NO2)4], (CN3H5)H[Co(MeNH2)2(NO2)4], [Co(MeNH2)3(NO2)3], [Co(MeNH2)3(NO2)2(NCS)], [Co(MeNH2)2(NH3)(NO2)3], [Co(MeNH2)4(NO2)2][Co(NH3)2(NO2)4] were prepared The complexes of MeNH2 are less stable than the analogous NH3 complexes.
IT 36741-31-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36741-31-8 CAPLUS
CN Cobalt, tris(methanamine)bis(nitrito-N)(thiocyanato-N)- (9CI) (CA INDEX NAME)



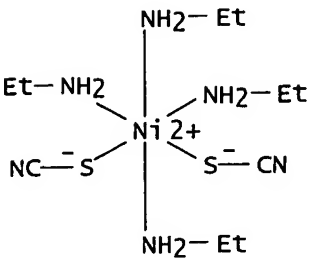
L10 ANSWER 44 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1971:544420 CAPLUS
DN 75:144420
TI Stepwise adduct formation of bis(O,O'-diethyldithiophosphato)nickel(II) with primary and secondary amines

AU Ciullo, G.; Furlani, C.; Sestili, L.; Sgamellotti, A.
CS Inst. Gen. Inorg. Chem., Univ. Perugia, Perugia, Italy
SO Inorganica Chimica Acta (1971), 5(3), 489-92
CODEN: ICHAA3; ISSN: 0020-1693
DT Journal
LA English
AB Bis(O,O'-diethyldithiophosphato)nickel(II) behaves in a qual. similar way with both primary and secondary amines in that 1:1 and 1:2 adducts are found. Data obtained for butylamine and diethylamine indicate that the difference in behavior towards primary and secondary amines is only quant., formation consts. being much smaller with the latter. Very high concn of primary amines leads also to the formation of complexes containing the chromophore (NiS2N4), presumably with monodentate dithiophosphate ligands.
IT 34406-41-2
RL: PRP (Properties); FORM (Formation, nonpreparative)
(formation consts. of)
RN 34406-41-2 CAPLUS
CN Nickel, tetrakis(butylamine)bis(dihydrogen phosphorodithioato)-, O,O,O,O-tetraethyl ester (8CI) (CA INDEX NAME)

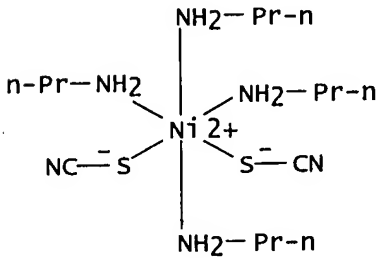


L10 ANSWER 45 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1970:91917 CAPLUS
DN 72:91917
TI Separation of aromatic hydrocarbons using metal-organic complexes
AU Csikos, Rezso; Farkas, Peter
CS Hung.
SO Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10, 107-16
CODEN: MAFKAJ; ISSN: 0506-807X
DT Journal
LA Hungarian
AB Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their selectivity, and stability were examined
IT 27910-87-8 27910-88-9 28067-98-3
RL: USES (Uses)
(in benzene derivative separation from heptane)
RN 27910-87-8 CAPLUS

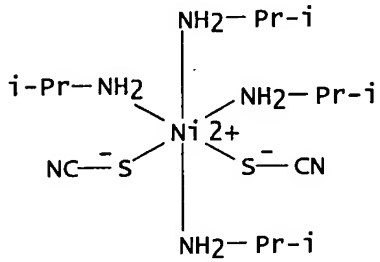
CN Nickel, tetrakis(ethylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)



RN 27910-88-9 CAPLUS
CN Nickel, tetrakis(propylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)

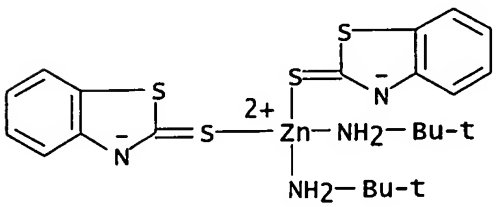


RN 28067-98-3 CAPLUS
CN Nickel, tetrakis(isopropylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)



L10 ANSWER 46 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1966:33012 CAPLUS
DN 64:33012
OREF 64:6075d
TI Vulcanization accelerator-activator complexes. I. Amine complexes of zinc and cadmium benzothiazole-2-thiolate
AU Milligan, Brian
CS Nat. Rubber Producers' Res. Assoc., Welwyn Garden City, UK
SO J. Chem. Soc., Inorg., Phys., Theoret. (1966), (1), 34-5
DT Journal
LA English
AB Eleven amine complexes of Zn benzothiazole-2-thiolate were prepared from the NH3 complex. Dissociation of the pyridine complex provides a convenient route

to the thiolate, which is difficult to prepare by other methods.
IT 15214-57-0P, Zinc, bis(2-benzothiazolethiolato)bis(tert-butylamine)-
RL: PREP (Preparation)
(preparation of)
RN 15214-57-0 CAPLUS
CN Zinc, bis(2(3H)-benzothiazolethionato-κS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)



=>
=>
Uploading C:\Program Files\Stnexp\Queries\10749450c.str

L11 STRUCTURE UPLOADED

=> d l11
L11 HAS NO ANSWERS
L11 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l11
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 05:07:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 81 TO ITERATE

100.0% PROCESSED 81 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1081 TO 2159
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L11

L13 0 L12

=> search l11
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 05:07:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 81 TO ITERATE

100.0% PROCESSED 81 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1081 TO 2159
PROJECTED ANSWERS: 0 TO 0

L14 0 SEA SSS SAM L11

L15 0 L14

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	645.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-34.50

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experimental property data in the original document. For information
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http://www.cas.org/ONLINE/UG/regprops.html

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=> s l11
SAMPLE SEARCH INITIATED 05:07:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       81 TO ITERATE

100.0% PROCESSED       81 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1081 TO     2159
PROJECTED ANSWERS:               0 TO        0

L16            0 SEA SSS SAM L11

=> search l11
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 05:07:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1257 TO ITERATE

100.0% PROCESSED     1257 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

L17            0 SEA SSS FUL L11

=> FIL STNGUIDE
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                        ENTRY     SESSION
FULL ESTIMATED COST                                     167.82      813.10

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
                                                        ENTRY     SESSION
CA SUBSCRIBER PRICE                                       0.00      -34.50

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Dec  8, 2006 (20061208/UP).

=> d his

     (FILE 'HOME' ENTERED AT 04:28:36 ON 11 DEC 2006)

     FILE 'REGISTRY' ENTERED AT 04:39:37 ON 11 DEC 2006
L1             STRUCTURE UPLOADED
L2           2 S L1
L3        1206 SEARCH L1 FULL
L4         791 S TRIFLATE
L5             STRUCTURE UPLOADED
L6           0 S L5
L7             STRUCTURE UPLOADED
L8           0 S L7
L9         121 SEARCH L7 FULL

     FILE 'CAPLUS' ENTERED AT 04:49:41 ON 11 DEC 2006
L10         46 S L9
L11            STRUCTURE UPLOADED
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                S L11

     FILE 'REGISTRY' ENTERED AT 05:07:25 ON 11 DEC 2006
L12             0 S L11

     FILE 'CAPLUS' ENTERED AT 05:07:26 ON 11 DEC 2006
L13             0 S L12
                S L11

     FILE 'REGISTRY' ENTERED AT 05:07:33 ON 11 DEC 2006
L14             0 S L11

     FILE 'CAPLUS' ENTERED AT 05:07:34 ON 11 DEC 2006
L15             0 S L14

     FILE 'REGISTRY' ENTERED AT 05:07:39 ON 11 DEC 2006
L16             0 S L11
L17             0 SEARCH L11 FULL

     FILE 'STNGUIDE' ENTERED AT 05:09:39 ON 11 DEC 2006

=> d l10 all
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:n


=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    1.26      814.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                    0.00      -34.50

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DICTIONARY FILE UPDATES:  10 DEC 2006  HIGHEST RN 915124-84-4

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d l9 1-121 all
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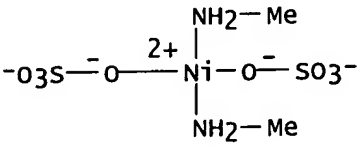
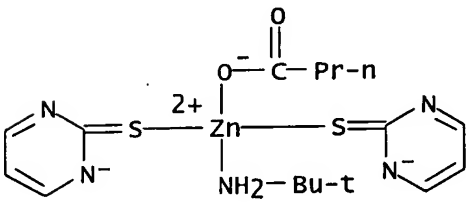
L9 ANSWER 1 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 791764-59-5 REGISTRY
ED Entered STN: 03 Dec 2004
CN Nickelate(2-), bis(methanamine)bis[sulfato(2-)-κO]- (9CI) (CA INDEX NAME)
MF C2 H10 N2 Ni O8 S2
CI CCS, COM
SR CA



L9 ANSWER 2 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 788144-09-2 REGISTRY
ED Entered STN: 25 Nov 2004
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyrimidinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 O2 S2 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4N2	NCNC3	6	C4N2	46.195.24	2

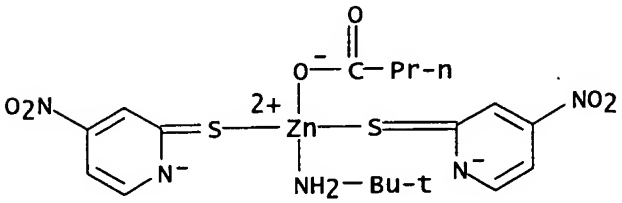


L9 ANSWER 3 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 774525-06-3 REGISTRY
ED Entered STN: 04 Nov 2004
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4-nitro-2(1H)-pyridinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C18 H24 N5 O6 S2 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence

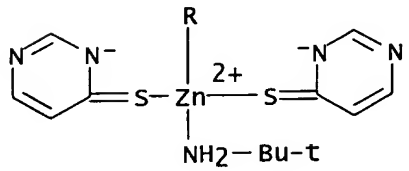
EA	ES	SZ	RF	RID	Count
C5N	NC5	6	C5N	46.156.21	2

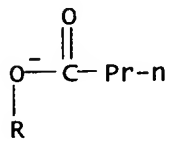


L9 ANSWER 4 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 767616-38-6 REGISTRY
ED Entered STN: 24 Oct 2004
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4(1H)-pyrimidinethionato-κS4)-, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 O2 S2 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4N2	NCNC3	6	C4N2	46.195.23	2



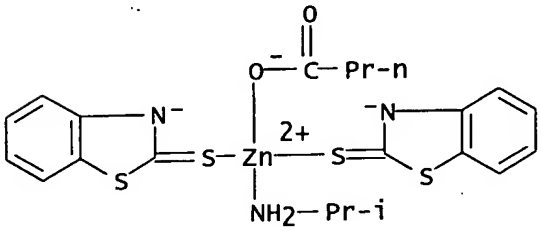


L9 ANSWER 5 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 765886-51-9 REGISTRY
ED Entered STN: 20 Oct 2004
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C21 H24 N3 O2 S4 Zn

CI CCS, COM
SR CA

Ring System Data

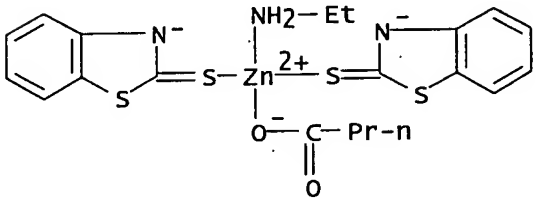
Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



L9 ANSWER 6 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 760160-39-2 REGISTRY
ED Entered STN: 11 Oct 2004
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(ethanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C20 H22 N3 O2 S4 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



L9 ANSWER 7 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 755740-20-6 REGISTRY
ED Entered STN: 01 Oct 2004
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C28 H34 N3 O2 S2 Zn

CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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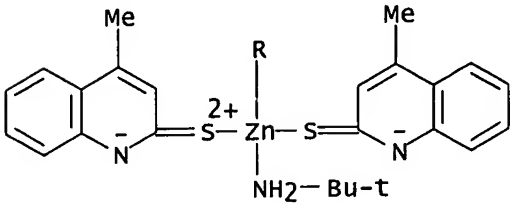
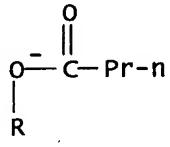
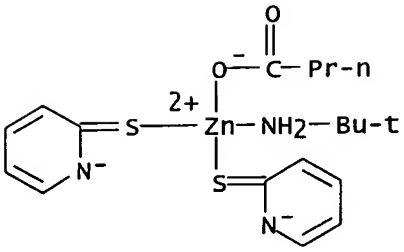




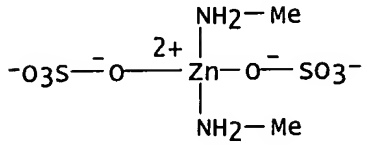
L9 ANSWER 8 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 750557-81-4 REGISTRY
ED Entered STN: 24 Sep 2004
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyridinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C18 H26 N3 O2 S2 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N	NC5	6	C5N	46.156.21	2



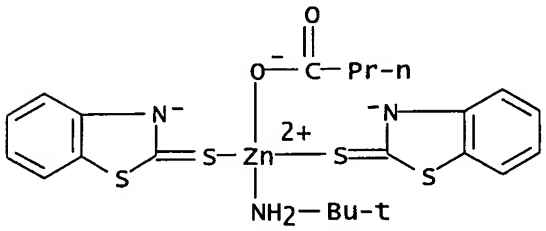
L9 ANSWER 9 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 745776-79-8 REGISTRY
ED Entered STN: 16 Sep 2004
CN Zincate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, (T-4)- (9CI) (CA INDEX NAME)
MF C2 H10 N2 O8 S2 Zn
CI CCS, COM
SR CA



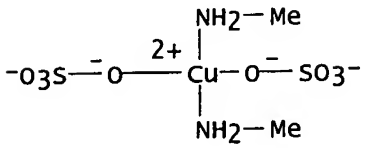
L9 ANSWER 10 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 742046-45-3 REGISTRY
ED Entered STN: 10 Sep 2004
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C22 H26 N3 O2 S4 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



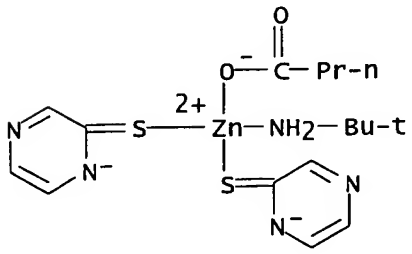
L9 ANSWER 11 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 742042-77-9 REGISTRY
ED Entered STN: 10 Sep 2004
CN Cuprate(2-), bis(methanamine)bis[sulfato(2-)-κO]- (9CI) (CA INDEX NAME)
MF C2 H10 Cu N2 O8 S2
CI CCS, COM
SR CA



L9 ANSWER 12 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 740072-13-3 REGISTRY
ED Entered STN: 05 Sep 2004
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyrazinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 O2 S2 Zn
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4N2	NC2NC2	6	C4N2	46.383.8	2



L9 ANSWER 13 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 713079-80-2 REGISTRY
ED Entered STN: 20 Jul 2004
CN Cadmium, bis(4-aminobenzenesulfonato-κO)tetrakis(1-propanamine)-, (OC-6-12)-, compd. with 1-propanamine (1:1) (9CI) (CA INDEX NAME)
MF C24 H48 Cd N6 O6 S2 . C3 H9 N
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2 in CM 1

CM 1

CRN 713079-79-9
CMF C24 H48 Cd N6 O6 S2
CCI CCS

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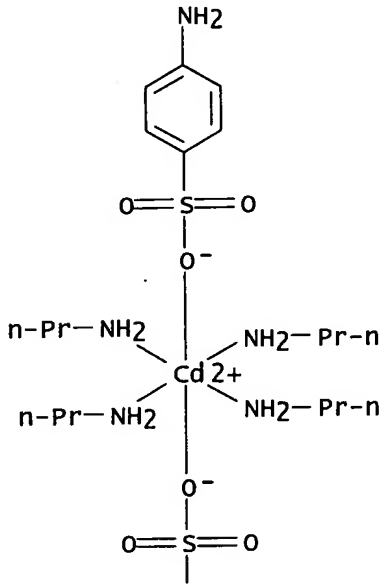

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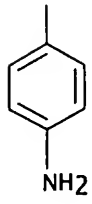
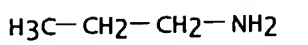


CM 2

CRN 107-10-8
CMF C3 H9 N



Experimental Property Tags (ETAG)

PROPERTY	NOTE
Crystal Structure	(1) CAS
IR Absorption Spectra	(1) CAS
Molecular Structure	(1) CAS

(1) Zhou, Jin-Sen; Dalton Transactions 2004(9) P1493-1497 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 141:81204 CA
TI Reversible and selective amine interactions of [Cd(μ2-N,O-p-NH2C6H4SO3)2(H2O)2]n
AU Zhou, Jin-Sen; Cai, Jiwen; Wang, Li; Ng, Seik-Weng
CS School of Chemistry & Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, Peop. Rep. China
SO Dalton Transactions (2004), (9), 1493-1497
CODEN: DTARAF; ISSN: 1477-9226
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
AB [Cd(μ2-N,O-p-NH2C6H4SO3)2(H2O)2]n (1) is a layered coordination compound The solid-vapor reactions between crystalline 1 and volatile amines were studied and the corresponding amine adducts were characterized by elemental anal., TGA, PXRD and IR. Among them, the C2H5NH2 and PrNH2 adducts, [Cd(C2H5NH2)4(H2O)2](H2NC6H4SO3)2 (3) and [Cd(PrNH2)4(O-p-H2NC6H4SO3)2]·PrNH2 (4), grew into single crystals in situ from the solid-vapor reaction processes and their crystal structures were characterized. In both cases, 4 mol equivalent of amine mols. coordinate to Cd(II) via replacing the N,O-p-NH2C6H4SO3 ligands or coordinated H2O mols. The single-phase product suggests that the solid-vapor reaction between the metal sulfonate and volatile alkylamines could be used as a green process to synthesize monoamine-coordinated Cd(II) complexes without any solvent and routine separation Finally, the substitution reaction is reversible at room conditions and selective for primary alkylamines.
ST crystal structure cadmium alkylamine aminobenzenesulfonate; substitution layered cadmium aminobenzenesulfonate aqua complex alkylamine vapor reversible; cadmium alkylamine aminobenzenesulfonate prepn structure; sulfanilate cadmium aqua complex solid substitution alkylamine vapor
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(aliphatic; reversible solid-vapor coordinative substitution of layered cadmium(II) aminobenzenesulfonate aqua solid with volatile alkylamines)

IT Crystal structure
Molecular structure
(of layered cadmium(II) aminobenzenesulfonate aqua complex and alkylamine-substituted derivs.)

IT Green chemistry
Substitution reaction, coordinative
(reversible solid-vapor coordinative substitution of layered cadmium(II) aminobenzenesulfonate aqua solid with volatile alkylamines)

IT 121-57-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of layered cadmium(II) aminobenzenesulfonate aqua complex and alkylamine-substituted derivs.)

IT 288855-36-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from dehydration of layered cadmium(II) aminobenzenesulfonate aqua complex)

IT 713079-78-8P 713079-80-2P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation via reversible solid-vapor coordinative substitution of layered cadmium(II) aminobenzenesulfonate aqua complex solid with volatile alkylamine, and crystal structure and TGA of)

IT 74-89-5DP, Methylamine, reaction product with cadmium(II) sulfanilate aqua complex 75-31-0DP, Isopropylamine, reaction product with cadmium(II) sulfanilate aqua complex 75-64-9DP, tert-Butylamine, reaction product with cadmium(II) sulfanilate aqua complex 78-81-9DP, Isobutylamine, reaction product with cadmium(II) sulfanilate aqua complex 109-73-9DP, n-Butylamine, reaction product with cadmium(II) sulfanilate aqua complex 713079-76-6DP, reaction products with alkylamines
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation via solid-vapor coordinative substitution of layered solid with volatile alkylamine, and TGA of)

IT 713079-76-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, layered crystal structure, dehydration, and reversible solid-vapor coordinative substitution with volatile alkylamines)

IT 74-89-5, Methylamine, reactions 75-04-7, Ethylamine, reactions 75-31-0, Isopropylamine, reactions 75-64-9, tert-Butylamine, reactions 78-81-9, Isobutylamine 107-10-8, n-Propylamine, reactions 109-73-9, n-Butylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reversible solid-vapor coordinative substitution of layered cadmium(II) aminobenzenesulfonate aqua complex solid with volatile alkylamine)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(2) Albrecht, M; J Chem Soc, Dalton Trans 2000, P3797 CAPLUS
(3) Albrecht, M; Nature 2000, V406, P970 CAPLUS
(4) Braga, D; Chem Commun 2001, P2272 CAPLUS
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L9 ANSWER 14 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 713079-79-9 REGISTRY
ED Entered STN: 20 Jul 2004
CN Cadmium, bis(4-aminobenzenesulfonato-κO)tetrakis(1-propanamine)-, (OC-6-12)- (9CI) (CA INDEX NAME)
MF C24 H48 Cd N6 O6 S2
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2

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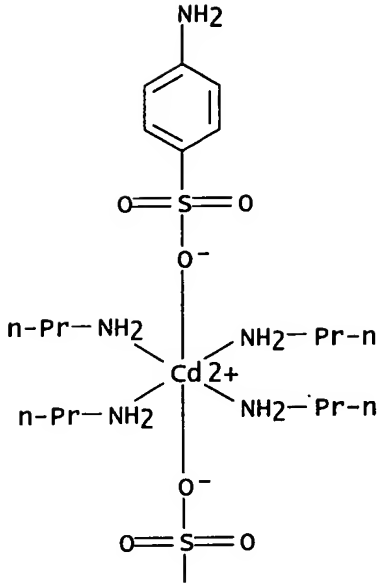

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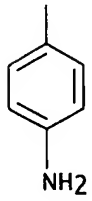
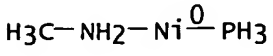


L9 ANSWER 15 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 682768-13-4 REGISTRY
ED Entered STN: 18 May 2004
CN Nickel, (methanamine)(phosphine)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (Methanamine)(phosphine)nickel
MF C H8 N Ni P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PRP (Properties)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 140:357466 CA
TI Theoretical studies on C-heteroatom bond formation via reductive elimination from group 10 M(PH3)2(CH3)(X) species (X = CH3, NH2, OH, SH) and the determination of metal-X bond strengths using density functional theory
AU MacGregor, Stuart A.; Neave, Greg W.; Smith, Christopher
CS Department of Chemistry, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK
SO Faraday Discussions (2003), 124, 111-127
CODEN: FDISE6; ISSN: 1359-6640
PB Royal Society of Chemistry
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22
AB D. functional calcns. were used to investigate C-C, C-N and C-O bond forming reactions via reductive elimination from Group 10 cis-[M(PH3)2(Me)(X)] species (X = Me, NH2, OH). Both direct reaction from the four-coordinate species and a three-coordinate mechanism involving initial PH3 loss was considered. For the four-coordinate pathway the ease of reductive elimination to give M(PH3)2 and Me-X follows the trend M = Pd < Pt < Ni. The reaction of the cis-M(PH3)2(Me)(NH2) species is promoted by the formation of methylamine adducts. Non-planar transition states are located and the C-heteroatom bond forming processes are characterized by migration of Me onto the cis-heteroatom ligand. For a given ligand, X, activation energies follow the trend M = Ni < Pd < Pt. Formation of the three-coordinate M(PH3)(Me)(X) species is promoted by a labilization of the cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OH. For the three-coordinate pathway the energy change for reductive elimination to give M(PH3) and Me-X again follows the trend M = Pd < Pt < Ni and in all cases the initial product is an M(PH3)(XMe) adduct. The three-coordinate transition states again involve migration of the Me ligand onto the cis-X ligand and for X = NH2 or OH activation energies follow the trend Ni > Pd < Pt. For a given metal activation energies in both the four- and three-coordinate pathways increase along the series Me < NH2 < OH. These trends in activation energy can be rationalized in terms of the strength of M-Me/M-X bonding as long as the extent of geometrical distortion required to obtain the transition state geometry is taken into account. Further calcns. on cis-Pd(PH3)2(Me)(SH) suggest that the more common exptl. observation of C(sp3)-S compared to C(sp3)-O reductive elimination arises from the greater kinetic accessibility of the former process rather than an intrinsic thermodn. preference for C-S bond formation. By comparison, the calcns. indicate that C(sp3)-N reductive elimination should be feasible from Ni and Pd systems. DF calcns. are shown to reproduce the relative homolytic bond strengths determined exptl. for Pt-X bonds. In the cis-M(PH3)2(Me)(X) systems the M-Me homolytic bond strength increases down the group while for M-NH2 and M-OH bonds the trend is M = Ni ≈ Pd < Pt. M-NH2 and M-OH bonds are considerably stronger than M-Me bonds and the presence of a heteroatom ligand serves to weaken M-CH3 bonds even further.
ST nickel palladium platinum phosphine methyl complex reductive elimination mechanism; Group 10 methyl alkoxy amido mercapto complex reductive elimination; reductive elimination DFT geometry Group 10 diphosphine methyl complex; activation energy DFT reductive elimination Group 10 methyl complex; transition state structure DFT reductive elimination methylnickel methylpalladium methylplatinum; mechanism four three

coordinate reductive elimination methylnickel methylpalladium methylplatinum

IT Bond energy
(DFT calcn. of homolytic bond strengths of Group 10 metals with carbon, nitrogen, oxygen an sulfur in reductive elimination from diphosphine complexes)

IT Density functional theory
Potential energy
(DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Group VIII element complexes
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(Group 10; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-carbon, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-nitrogen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-oxygen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-sulfur; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Molecular structure
(optimized; of nickel, palladium and platinum Me amido-, alkoxy- and mercapto-complexes)

IT Activation energy
Transition state structure
(reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Elimination reaction, coordinative
(reductive; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Coordination number
(three; comparison of three- and four-coordinate pathway of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes by DFT geometry and energy profile calcn.)

IT 682768-21-4, (Methanethiol)(phosphine)palladium
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 682767-97-1, (Methanamine)bis(phosphine)nickel 682767-98-2, (Methanamine)bis(phosphine)palladium 682767-99-3, (Methanamine)bis(phosphine)platinum 682768-00-9, (Methanol)bis(phosphine)nickel
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(optimized geometry, potential energy, dissociation; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 67-56-1, Methanol, properties 74-84-0, Ethane, properties 74-89-5,

Methanamine, properties 66048-71-3, Bis(phosphine)nickel 76830-85-8, Bis(phosphine)platinum 78452-79-6, Bis(phosphine)palladium 682768-10-1 682768-11-2 682768-12-3 682768-13-4, (Methanamine)(phosphine)nickel 682768-14-5, (Methanamine)(phosphine)palladium 682768-15-6, (Methanamine)(phosphine)platinum 682768-16-7, (Methanol)(phosphine)nickel 682768-17-8, (Methanol)(phosphine)palladium 682768-18-9, (Methanol)(phosphine)platinum 682768-20-3, (Methanethiol)bis(phosphine)palladium
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 79218-09-0, Dimethyl(phosphine)palladium 682768-02-1, Dimethyl(phosphine)nickel 682768-03-2, Dimethyl(phosphine)platinum 682768-04-3, (Amido)(methyl)(phosphine)nickel 682768-05-4, (Amido)(methyl)(phosphine)palladium 682768-06-5, (Amido)(methyl)(phosphine)platinum 682768-07-6, (Hydroxo)(methyl)(phosphine)nickel 682768-08-7, (Hydroxo)(methyl)(phosphine)palladium 682768-09-8, (Hydroxo)(methyl)(phosphine)platinum 682768-19-0
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 79218-06-7 79218-07-8 79232-18-1 682767-91-5, cis-(Amido)methylbis(phosphine)nickel 682767-92-6, cis-(Amido)methylbis(phosphine)palladium 682767-93-7, cis-(Amido)methylbis(phosphine)platinum 682767-94-8, cis-(Hydroxo)methylbis(phosphine)nickel 682767-95-9, cis-(Hydroxo)methylbis(phosphine)palladium 682767-96-0, cis-(Hydroxo)methylbis(phosphine)platinum 682768-01-0
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

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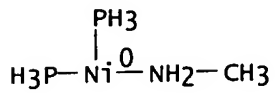
RN 682767-97-1 REGISTRY
ED Entered STN: 18 May 2004
CN Nickel, (methanamine)bis(phosphine)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (Methanamine)bis(phosphine)nickel
MF C H11 N Ni P2
CI CCS

SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 140:357466 CA
TI Theoretical studies on C-heteroatom bond formation via reductive elimination from group 10 M(PH3)2(CH3)(X) species (X = CH3, NH2, OH, SH) and the determination of metal-X bond strengths using density functional theory
AU MacGregor, Stuart A.; Neave, Greg W.; Smith, Christopher
CS Department of Chemistry, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK
SO Faraday Discussions (2003), 124, 111-127
CODEN: FDISE6; ISSN: 1359-6640
PB Royal Society of Chemistry
DT Journal
LA English
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22
AB D. functional calcns. were used to investigate C-C, C-N and C-O bond forming reactions via reductive elimination from Group 10 cis-[M(PH3)2(Me)(X)] species (X = Me, NH2, OH). Both direct reaction from the four-coordinate species and a three-coordinate mechanism involving initial PH3 loss was considered. For the four-coordinate pathway the ease of reductive elimination to give M(PH3)2 and Me-X follows the trend M = Pd < Pt < Ni. The reaction of the cis-M(PH3)2(Me)(NH2) species is promoted by the formation of methylamine adducts. Non-planar transition states are located and the C-heteroatom bond forming processes are characterized by migration of Me onto the cis-heteroatom ligand. For a given ligand, X, activation energies follow the trend M = Ni < Pd < Pt. Formation of the three-coordinate M(PH3)(Me)(X) species is promoted by a labilization of the cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OH. For the three-coordinate pathway the energy change for reductive elimination to give M(PH3) and Me-X again follows the trend M = Pd < Pt < Ni and in all cases the initial product is an M(PH3)(XMe) adduct. The three-coordinate transition states again involve migration of the Me ligand onto the cis-X ligand and for X = NH2 or OH activation energies follow the trend Ni > Pd < Pt. For a given metal activation energies in both the four- and three-coordinate pathways increase along the series Me < NH2 < OH. These trends in activation energy can be rationalized in terms of the strength of M-Me/M-X bonding as long as the extent of geometrical distortion required to obtain the transition state geometry is taken into account. Further calcns. on cis-Pd(PH3)2(Me)(SH) suggest that the more common exptl. observation of C(sp3)-S compared to C(sp3)-O reductive elimination arises from the greater kinetic accessibility of the former process rather than an intrinsic thermodn. preference for C-S bond formation. By comparison, the calcns. indicate that C(sp3)-N reductive elimination should be feasible from Ni and Pd systems. DF calcns. are

shown to reproduce the relative homolytic bond strengths determined exptl. for Pt-X bonds. In the cis-M(PH3)2(Me)(X) systems the M-Me homolytic bond strength increases down the group while for M-NH2 and M-OH bonds the trend is M = Ni ≈ Pd < Pt. M-NH2 and M-OH bonds are considerably stronger than M-Me bonds and the presence of a heteroatom ligand serves to weaken M-CH3 bonds even further.

ST nickel palladium platinum phosphine methyl complex reductive elimination mechanism; Group 10 methyl alkoxy amido mercapto complex reductive elimination; reductive elimination DFT geometry Group 10 diphosphine methyl complex; activation energy DFT reductive elimination Group 10 methyl complex; transition state structure DFT reductive elimination methylnickel methylpalladium methylplatinum; mechanism four three coordinate reductive elimination methylnickel methylpalladium methylplatinum

IT Bond energy
(DFT calcn. of homolytic bond strengths of Group 10 metals with carbon, nitrogen, oxygen an sulfur in reductive elimination from diphosphine complexes)

IT Density functional theory
Potential energy
(DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Group VIII element complexes
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(Group 10; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-carbon, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-nitrogen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-oxygen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Bond formation
(carbon-sulfur; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Molecular structure
(optimized; of nickel, palladium and platinum Me amido-, alkoxy- and mercapto-complexes)

IT Activation energy
Transition state structure
(reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Elimination reaction, coordinative
(reductive; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT Coordination number
(three; comparison of three- and four-coordinate pathway of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes by DFT geometry and energy profile calcn.)

IT 682768-21-4, (Methanethiol)(phosphine)palladium
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 682767-97-1, (Methanamine)bis(phosphine)nickel 682767-98-2, (Methanamine)bis(phosphine)palladium 682767-99-3, (Methanamine)bis(phosphine)platinum 682768-00-9, (Methanol)bis(phosphine)nickel
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(optimized geometry, potential energy, dissociation; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 67-56-1, Methanol, properties 74-84-0, Ethane, properties 74-89-5, Methanamine, properties 66048-71-3, Bis(phosphine)nickel 76830-85-8, Bis(phosphine)platinum 78452-79-6, Bis(phosphine)palladium 682768-10-1 682768-11-2 682768-12-3 682768-13-4, (Methanamine)(phosphine)nickel 682768-14-5, (Methanamine)(phosphine)palladium 682768-15-6, (Methanamine)(phosphine)platinum 682768-16-7, (Methanol)(phosphine)nickel 682768-17-8, (Methanol)(phosphine)palladium 682768-18-9, (Methanol)(phosphine)platinum 682768-20-3, (Methanethiol)bis(phosphine)palladium
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 79218-09-0, Dimethyl(phosphine)palladium 682768-02-1, Dimethyl(phosphine)nickel 682768-03-2, Dimethyl(phosphine)platinum 682768-04-3, (Amido)(methyl)(phosphine)nickel 682768-05-4, (Amido)(methyl)(phosphine)palladium 682768-06-5, (Amido)(methyl)(phosphine)platinum 682768-07-6, (Hydroxo)(methyl)(phosphine)nickel 682768-08-7, (Hydroxo)(methyl)(phosphine)palladium 682768-09-8, (Hydroxo)(methyl)(phosphine)platinum 682768-19-0
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

IT 79218-06-7 79218-07-8 79232-18-1 682767-91-5, cis-(Amido)methylbis(phosphine)nickel 682767-92-6, cis-(Amido)methylbis(phosphine)palladium 682767-93-7, cis-(Amido)methylbis(phosphine)platinum 682767-94-8, cis-(Hydroxo)methylbis(phosphine)nickel 682767-95-9, cis-(Hydroxo)methylbis(phosphine)palladium 682767-96-0, cis-(Hydroxo)methylbis(phosphine)platinum 682768-01-0
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)

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L9 ANSWER 17 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-20-2 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(2-methyl-1-propanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with 2-methyl-1-propanamine (1:1), dihydrate (9CI) (CA INDEX NAME)
MF C18 H28 Cd N2 O6 S2 . C4 H11 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1 in CM 1

CM 1

CRN 595548-19-9
CMF C18 H28 Cd N2 O6 S2
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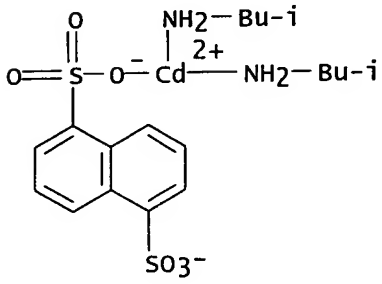
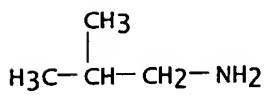


CM 2

CRN 78-81-9
CMF C4 H11 N



Experimental Property Tags (ETAG)

PROPERTY	NOTE
IR Spectra	(1) CAS
X-Ray Diffraction Pattern	(1) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811
CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:239001 CA
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.
ST cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
IT Thermal decomposition
(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT Intercalation
(selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 595548-08-6P 595548-10-0P 595548-12-2P 595548-14-4P 595548-16-6P
595548-18-8P 595548-20-2P 595548-21-3P 595548-22-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)
IT 473251-23-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 81-04-9, 1,5-Naphthalenedisulfonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
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(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
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(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
(16) Eddoudi, M; Acc Chem Res 2001, V34, P319
(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Commun 2003, P854 CAPLUS
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
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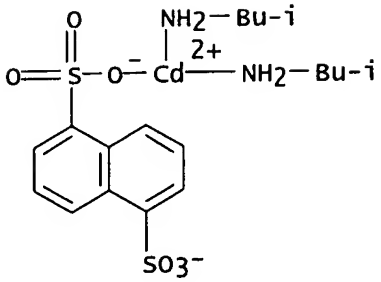
L9 ANSWER 18 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-19-9 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(2-methyl-1-propanamine)[1,5-naphthalenedisulfonato(2-)-κO]- (9CI) (CA INDEX NAME)
MF C18 H28 Cd N2 O6 S2
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1



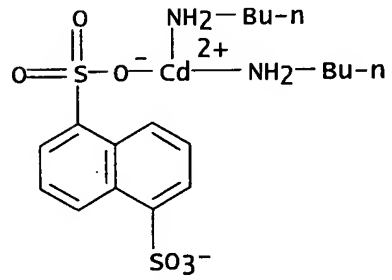
L9 ANSWER 19 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-18-8 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(1-butanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with 1-butanamine (1:1), dihydrate (9CI) (CA INDEX NAME)
MF C18 H28 Cd N2 O6 S2 . C4 H11 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1 in CM 1

CM 1

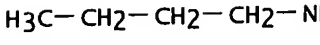
CRN 595548-17-7
CMF C18 H28 Cd N2 O6 S2
CCI CCS



CM 2

CRN 109-73-9

CMF C4 H11 N



Experimental Property Tags (ETAG)

PROPERTY	NOTE
IR Spectra	(1) CAS
X-Ray Diffraction Pattern	(1) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811
CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:239001 CA
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.
ST cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
IT Thermal decomposition
(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT Intercalation
(selective amine coordinative substitution/intercalation behavior of

cadmium diaqua naphthalenedisulfonate complex)
IT 595548-08-6P 595548-10-0P 595548-12-2P 595548-14-4P 595548-16-6P
595548-18-8P 595548-20-2P 595548-21-3P 595548-22-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)
IT 473251-23-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 81-04-9, 1,5-Naphthalenedisulfonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
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(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
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(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
(16) Eddoudi, M; Acc Chem Res 2001, V34, P319
(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
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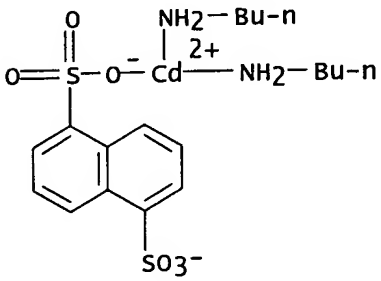
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
(30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
(35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS

L9 ANSWER 20 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-17-7 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(1-butanamine)[1,5-naphthalenedisulfonato(2-)-κO]- (9CI) (CA INDEX NAME)
MF C18 H28 Cd N2 O6 S2
CI CCS, COM

SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1



L9 ANSWER 21 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-16-6 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(2-propanamine)-, compd. with 2-propanamine (1:1), dihydrate (9CI) (CA INDEX NAME)
MF C16 H24 Cd N2 O6 S2 . C3 H9 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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CM 1

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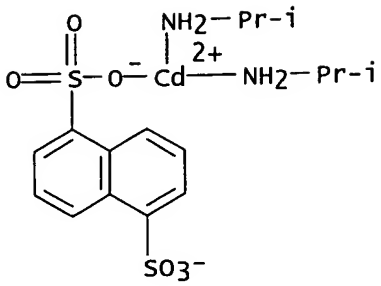
CCI CCS



CM 2

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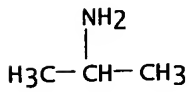

Experimental Property Tags (ETAG)

PROPERTY	NOTE
IR Spectra	(1) CAS
X-Ray Diffraction Pattern	(1) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811
CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

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TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
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CC 78-3 (Inorganic Chemicals and Reactions)
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were

intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.

ST cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation

IT Thermal decomposition
(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)

IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

IT Intercalation
(selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

IT 595548-08-6P 595548-10-0P 595548-12-2P 595548-14-4P 595548-16-6P
595548-18-8P 595548-20-2P 595548-21-3P 595548-22-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)

IT 473251-23-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

IT 81-04-9, 1,5-Naphthalenedisulfonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
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(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
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(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
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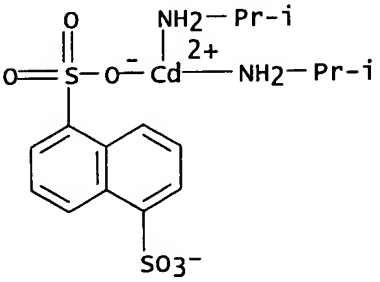
(25) Pan, L; Chem Commun 2003, P854 CAPLUS

(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
(30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
(35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS

L9 ANSWER 22 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-15-5 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(2-propanamine)-(9CI) (CA INDEX NAME)
MF C16 H24 Cd N2 O6 S2
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1



L9 ANSWER 23 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-14-4 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(1-propanamine)-, compd. with 1-propanamine (1:2), dihydrate (9CI) (CA INDEX NAME)
MF C16 H24 Cd N2 O6 S2 . 2 C3 H9 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

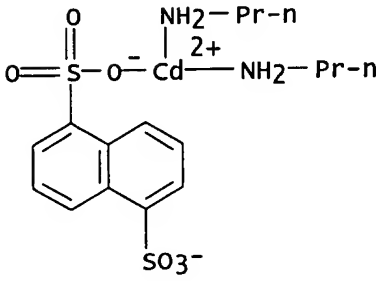
Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count

C6-C6	C6-C6	6-6	C10	591.49.57	1 in CM 1

CM 1

CRN 595548-13-3
CMF C16 H24 Cd N2 O6 S2
CCI CCS



CM 2

CRN 107-10-8
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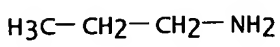


Experimental Property Tags (ETAG)

PROPERTY	NOTE
IR Spectra	(1) CAS
X-Ray Diffraction Pattern	(1) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811
CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:239001 CA
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry

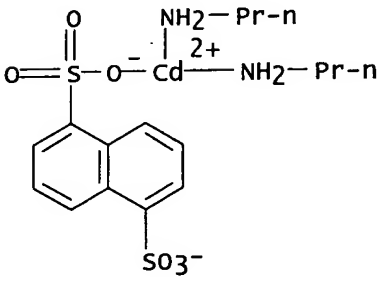
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.
ST cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
IT Thermal decomposition
(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT Intercalation
(selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 595548-08-6P 595548-10-0P 595548-12-2P 595548-14-4P 595548-16-6P
595548-18-8P 595548-20-2P 595548-21-3P 595548-22-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)
IT 473251-23-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 81-04-9, 1,5-Naphthalenedisulfonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
(16) Eddoudi, M; Acc Chem Res 2001, V34, P319

(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Commun 2003, P854 CAPLUS
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
(30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
(35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS

L9 ANSWER 24 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-13-3 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(1-propanamine)-(9CI) (CA INDEX NAME)
MF C16 H24 Cd N2 O6 S2
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1



L9 ANSWER 25 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-12-2 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(ethanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with ethanamine (1:2), dihydrate (9CI) (CA INDEX NAME)
MF C14 H20 Cd N2 O6 S2 . 2 C2 H7 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal

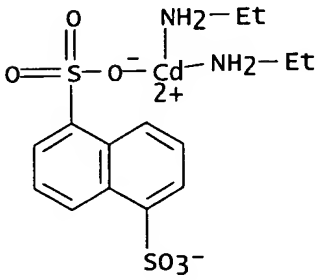
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1 in CM 1

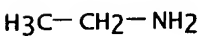
CM 1

CRN 595548-11-1
CMF C14 H20 Cd N2 O6 S2
CCI CCS



CM 2

CRN 75-04-7
CMF C2 H7 N



Experimental Property Tags (ETAG)

PROPERTY	NOTE
IR Spectra	(1) CAS
X-Ray Diffraction Pattern	(1) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

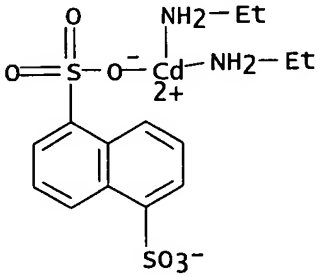
AN 139:239001 CA
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.
ST cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
IT Thermal decomposition
(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT Intercalation
(selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 595548-08-6P 595548-10-0P 595548-12-2P 595548-14-4P 595548-16-6P
595548-18-8P 595548-20-2P 595548-21-3P 595548-22-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)
IT 473251-23-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 81-04-9, 1,5-Naphthalenedisulfonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS

(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
(16) Eddoudi, M; Acc Chem Res 2001, V34, P319
(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Commun 2003, P854 CAPLUS
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
(30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
(35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS

L9 ANSWER 26 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-11-1 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(ethanamine)[1,5-naphthalenedisulfonato(2-)-κO]- (9CI) (CA INDEX NAME)
MF C14 H20 Cd N2 O6 S2
CI CCS, COM
SR CA

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1



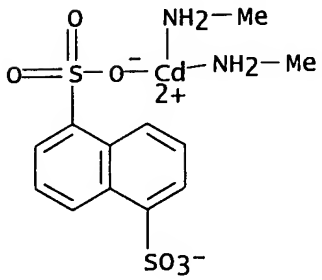
L9 ANSWER 27 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-10-0 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(methanamine)[1,5-naphthalenedisulfonato(2-)-κO]-, compd. with methanamine (1:1), dihydrate (9CI) (CA INDEX NAME)
MF C12 H16 Cd N2 O6 S2 . C H5 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1 in CM 1

CM 1

CRN 595548-09-7
CMF C12 H16 Cd N2 O6 S2
CCI CCS



CM 2

CRN 74-89-5
CMF C H5 N

Experimental Property Tags (ETAG)

PROPERTY	NOTE
IR Spectra	(1) CAS
X-Ray Diffraction Pattern	(1) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811
CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:239001 CA
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.
ST cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
IT Thermal decomposition
(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT Intercalation
(selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 595548-08-6P 595548-10-0P 595548-12-2P 595548-14-4P 595548-16-6P
595548-18-8P 595548-20-2P 595548-21-3P 595548-22-4P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)
IT 473251-23-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)
IT 81-04-9, 1,5-Naphthalenedisulfonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
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(9) Chui, S; Science 1999, V283, P1148 CAPLUS
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(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
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(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
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(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
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(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
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(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
(35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS

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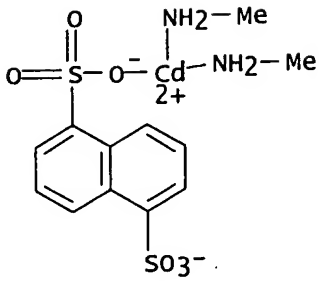
RN 595548-09-7 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(methanamine)[1,5-naphthalenedisulfonato(2-)-κO]- (9CI)
(CA INDEX NAME)
MF C12 H16 Cd N2 O6 S2
CI CCS, COM
SR CA

Ring System Data

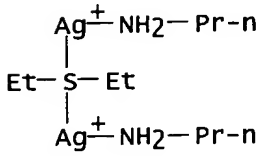
Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6-C6	C6-C6	6-6	C10	591.49.57	1



L9 ANSWER 29 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 550305-04-9 REGISTRY
ED Entered STN: 18 Jul 2003
CN Silver(2+), bis(1-propanamine)[μ-[1,1'-thiobis[ethane]]]di-, dinitrite (9CI) (CA INDEX NAME)
MF C10 H28 Ag2 N2 S . 2 N O2
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

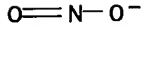
CM 1

CRN 550305-03-8
CMF C10 H28 Ag2 N2 S
CCI CCS



CM 2

CRN 14797-65-0
CMF N O2



Experimental Property Tags (ETAG)

PROPERTY	NOTE
Proton NMR Spectra	(1) CAS

(1) Jung, Won Cheol; EP 1323721 A2 2003 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:77881 CA
TI Metal thioether complexes as organic metal precursors for use in forming metal-containing patterned films
IN Jung, Won Cheol; Chang, Seok; Hwang, Soon Taik; Byun, Young Hun
PA Samsung Electronics Co., Ltd., S. Korea
SO Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DT Patent
LA English
IC ICM C07F001-00
ICS C07F003-00; C07F015-00; C07F015-06; C07F015-04; C23C016-00
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 74
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1323721	A2	20030702	EP 2002-257784	20021111
	EP 1323721	A3	20031008		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	KR 2003057133	A	20030704	KR 2001-87510	20011228
	US 2003124457	A1	20030703	US 2002-282031	20021029
	US 6965045	B2	20051115		
	JP 2003286579	A2	20031010	JP 2002-373621	20021225
PRAI	KR 2001-87510		20011228		

AB Disclosed are organic metal precursors comprising one or more thioether ligands bonded to one or more metal atoms (metal = Ag, Au, Co, Cu, Pd, Ni, Pt, Zn, Cd), wherein the organic ligand is rapidly dissociated from the metal atom upon exposure to light and degraded leaving a metal or a metal oxide. Thus, reaction of AgNO2 and Et2S in heated MeCN afforded [(Et2S)Ag+](NO2-). Reaction of the latter with PrNH2 in MeCN afforded [(PrNH2)Ag]2SEt2. Using the organic metal precursors of the present invention, e.g., [(PrNH2)Ag]2SEt2, an electroconductive, metal-containing patterned film can be easily deposited on a substrate at room temperature under atmospheric pressure without using photosensitive resins.

ST transition metal thioether complex prepn photodegrdn; patterned silver film prepn photodegrdn thioether complex precursor; silver thioether complex prepn photodegrdn patterned film precursor

IT Films
(elec. conductive, patterned; preparation of metal thioether complexes and their photodegrdn. to form metal-containing patterned films without use of photosensitive resins)

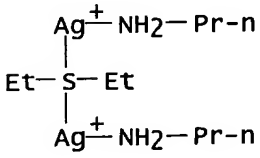
IT Electric conductors
(films, patterned; preparation of metal thioether complexes and their photodegrdn. to form metal-containing patterned films without use of photosensitive resins)

IT Transition metal complexes
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(thioether; preparation of metal thioether complexes and their photodegrdn. to form metal-containing patterned films without use of photosensitive resins)

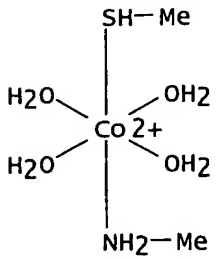
IT 107-10-8, Propylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with silver thioether complex to give precursor of

silver-containing patterned films)
IT 60-29-7, Diethyl ether, reactions 110-01-0, Tetrahydrothiophene
7761-88-8, Silver nitrate, reactions 7783-99-5, Silver nitrite
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation with thioethers to give precursors of silver-containing patterned films)
IT 550304-99-9P 550305-01-6P 550305-02-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation as precursor for use in forming metal-containing patterned film)
IT 550305-04-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation as precursor for use in forming metal-containing patterned film via photodegrdn. without use of photosensitive resins)

L9 ANSWER 30 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 550305-03-8 REGISTRY
ED Entered STN: 18 Jul 2003
CN Silver(2+), bis(1-propanamine)[μ-[1,1'-thiobis[ethane]]]di- (9CI) (CA INDEX NAME)
MF C10 H28 Ag2 N2 S
CI CCS, COM
SR CA



L9 ANSWER 31 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 284476-55-7 REGISTRY
ED Entered STN: 09 Aug 2000
CN Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-23)- (9CI) (CA INDEX NAME)
MF C2 H17 Co N O4 S
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 133:125569 CA
TI Ab Initio calculations of [CoY6-nXn]2+ complexes
AU Rulisek, Lubomir; Havlas, Zdenek
CS Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic, Prague, 166 10, Czech Rep.
SO Journal of Chemical Physics (2000), 112(1), 149-157
CODEN: JCPSA6; ISSN: 0021-9606
PB American Institute of Physics
DT Journal
LA English
CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 6, 68, 78
AB The CASSCF and multi-reference second order perturbation theory (CASPT2) calcns. of [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes (X = CH3OH, CH3SH, CH3NH2) are reported. The potential energy surfaces of 10 lowest quartet states of [Co(H2O)5X]2+ complexes near the equilibrium geometry are calculated and splitting of triple-degenerate 4T1g(F), 4T2g(F), and 4T1g(P) electronic states of [Co(H2O)6]2+ complex induced by the substitution of one or two water ligands is characterized and quantified. The energy differences between originally degenerate states are almost invariant to the changes of metal-ligand distances, and despite their proximity, the crossing does not occur. The coeffs. of the leading configuration of multi-reference wave functions of [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes are shown to approach unity and the usage of single-reference methods is justified. As a consequence, interaction energies of the studied functional groups with Co2+ are computed also at the HF, DFT and MP2 levels. They are compared to CASSCF calcns. and to the equivalent calcns. done for Zn2+ and Ni2+ ions. The computational methodol. for the accurate calcns. of various cobalt (II) ionic complexes is described and the implications for the theor. investigation of interactions of chemical and biol. important functional groups with Co2+ are discussed.
ST cobalt mixed ligand complex CASSCF CASPT2 HF MP2 DFT; potential surface cobalt mixed ligand complex; quartet state PES cobalt mixed ligand complex; degenerate state cobalt mixed ligand complex PES; fluoride cobalt complex electronic structure geometry; water mixed ligand complex cobalt electronic structure geometry; ammonia mixed ligand complex cobalt electronic structure geometry; methylamine mixed ligand complex cobalt electronic structure geometry; methanol mixed ligand complex cobalt electronic structure geometry; methanethiol mixed ligand complex cobalt electronic structure geometry
IT Bond length
Electronic excitation
Energy level splitting
Ground state
Jahn-Teller effect
Molecular structure
Potential energy surface
(ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))
IT Electronic state
(quartet; ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))
IT Energy

(substitution-reaction; ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))

IT 15276-47-8, Hexaaquacobalt(2+) 15365-75-0, Hexaamminecobalt(2+) 29858-93-3 29868-74-4, Hexafluorocobaltate(4-) 60119-04-2 60119-05-3 79231-71-3 125823-87-2 223243-89-8 223243-91-2 282542-77-2 282547-96-0 282547-97-1 282549-07-9 282550-54-3 284476-55-7 284476-56-8 284476-58-0
RL: PRP (Properties)
(ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))

RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD

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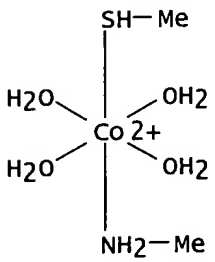
L9 ANSWER 32 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 282547-96-0 REGISTRY
ED Entered STN: 02 Aug 2000
CN Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-32)- (9CI) (CA INDEX NAME)
MF C2 H17 Co N O4 S
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE 1

AN 133:125569 CA
TI Ab Initio calculations of [CoY6-nXn]2+ complexes
AU Rulisek, Lubomir; Havlas, Zdenek
CS Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic, Prague, 166 10, Czech Rep.
SO Journal of Chemical Physics (2000), 112(1), 149-157
CODEN: JCPSA6; ISSN: 0021-9606
PB American Institute of Physics
DT Journal
LA English
CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 6, 68, 78

AB The CASSCF and multi-reference second order perturbation theory (CASPT2) calcns. of [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes (X = CH3OH, CH3SH, CH3NH2) are reported. The potential energy surfaces of 10 lowest quartet states of [Co(H2O)5X]2+ complexes near the equilibrium geometry are calculated and splitting of triple-degenerate 4T1g(F), 4T2g(F), and 4T1g(P) electronic states of [Co(H2O)6]2+ complex induced by the substitution of one or two water ligands is characterized and quantified. The energy differences between originally degenerate states are almost invariant to the changes of metal-ligand distances, and despite their proximity, the crossing does not occur. The coeffs. of the leading configuration of multi-reference wave functions of [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes are shown to approach unity and the usage of single-reference methods is justified. As a consequence, interaction energies of the studied functional groups with Co2+ are computed also at the HF, DFT and MP2 levels. They are compared to CASSCF calcns. and to the equivalent calcns. done for Zn2+ and Ni2+ ions. The computational methodol. for the accurate calcns. of various cobalt (II) ionic complexes is described and the implications for the theor. investigation of interactions of chemical and biol. important functional groups with Co2+ are discussed.

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Ground state
Jahn-Teller effect
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Potential energy surface
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IT Electronic state
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IT 15276-47-8, Hexaaquacobalt(2+) 15365-75-0, Hexaamminecobalt(2+)
29858-93-3 29868-74-4, Hexafluorocobaltate(4-) 60119-04-2 60119-05-3
79231-71-3 125823-87-2 223243-89-8 223243-91-2 282542-77-2
282547-96-0 282547-97-1 282549-07-9 282550-54-3 284476-55-7
284476-56-8 284476-58-0
RL: PRP (Properties)
(ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))

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L9 ANSWER 33 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 279674-00-9 REGISTRY
ED Entered STN: 24 Jul 2000
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κO]-, (OC-6-23)-, perchlorate (9CI) (CA INDEX NAME)
MF C H17 Co N5 O4 S . Cl O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)

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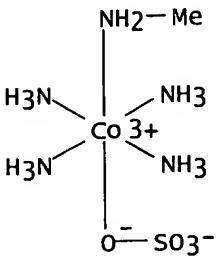
CRN 210574-34-8
CMF C H17 Co N5 O4 S
CCI CCS



CM 2

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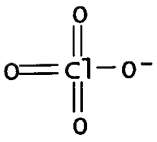
CMF Cl O4



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 133:79995 CA
TI Inductive effect of methyl groups on acidopentaaminecobalt(III) complexes
AU Benzo, Fabian; Beyer, Lothar; Bozoglian, Fernando; Hallmeier, Karl-Heinz; Sienra, Beatriz
CS Universidad de la Republica, Catedra de Quimica Inorganica, Montevideo, Urug.
SO Polyhedron (2000), 19(8), 971-974
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal

LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB Electron spectroscopy for chemical anal. (ESCA) was performed for [Co(NH3)5Cl](Clo4)2, trans-[Co(NH3)4(NH2CH3)Cl]-(Clo4) 2, [Co(NH2CH3)5Cl](Clo4)2 and trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) complexes. Comparison of the results for the complexes [Co(NH3)5Cl](Clo4)2 and trans-[Co(NH3)4(NH2CH3)Cl](Clo4)2 shows clearly the electronic influence (+I effect) of the methylamine group on the cobalt and through this on the chlorine atom in trans position. Comparison of [Co(NH2CH3)5Cl](Clo4)2 with trans-[Co(NH3)4(NH2CH3)Cl](Clo4)2 shows that methylation of the four cis-NH3 ligands does not produce a proportional decrease in the binding energy of the cobalt atom, while the electron d. of the chloro ligand is not affected. For the complex trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) the +I effect is almost completely compensated by the presence of the sulfato group in trans position. Acid dissociation consts. are also reported for [Co(NH3)5(OH2)]3+ and trans-[Co(NH3)4(NH2CH3)(OH2)]3 + ions. The implications of these results for the mechanism of the acid and base hydrolysis reactions of acidopentaaminecobalt(III) complexes are discussed. The preparation of the trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) complex through the trans-[Co(NH3)4(NH2CH3)(SO3)]+ precursor is also described.
ST inductive effect methyl group acido amine cobalt complex
IT Hydrolysis
(acid, mechanism; inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT Dissociation constant
(acid; inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT Hydrolysis
(base, mechanism; inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT Inductive effect
Methyl group
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT 15156-18-0 15392-60-6 91321-36-7 279674-00-9
RL: PRP (Properties)
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT 14403-82-8 68250-09-9 134066-32-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
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L9 ANSWER 34 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-83-3 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zinc, bis(4,6-dimethyl-2(1H)-pyrimidinethionato-κS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C20 H36 N6 S2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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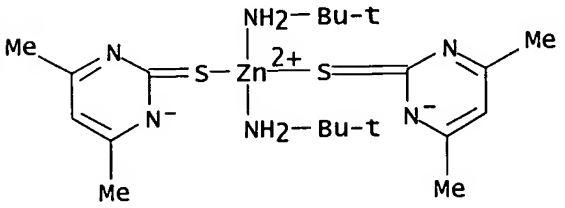

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475

PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)
AB Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
ST sulfur vulcanization SBR quant structure property relationship
IT Molecular structure-property relationship
Sulfidation
Vulcanization
Vulcanization accelerators and agents
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, Sulfur, uses
10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
156017-14-0 156477-90-6 157993-40-3 188036-96-6 252564-20-8
252564-21-9 252564-22-0 252564-23-1 252564-24-2 252564-25-3
252564-26-4 252564-27-5 252564-28-6 252564-29-7 252564-30-0
252564-31-1 252564-32-2 252564-33-3 252564-34-4 252564-35-5
252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)
RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
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L9 ANSWER 35 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-38-8 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-methyl-2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C22 H26 N3 O2 S4 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (742046-45-3)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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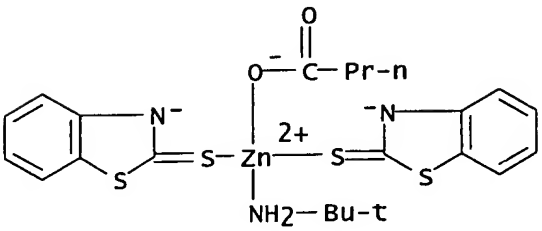

● H+

1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)

AB Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.

ST sulfur vulcanization SBR quant structure property relationship

IT Molecular structure-property relationship
Sulfidation
Vulcanization
Vulcanization accelerators and agents
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, sulfur, uses
10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
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252564-31-1 252564-32-2 252564-33-3 252564-34-4 252564-35-5
252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Anon; Natural Rubber Science and Technology 1988, P570
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(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
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(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-, and Cosmosphere Technology 1984, V5, P31
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(41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267 CAPLUS
(47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
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(53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
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(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
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RN 252564-37-7 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyrimidinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 O2 S2 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (788144-09-2)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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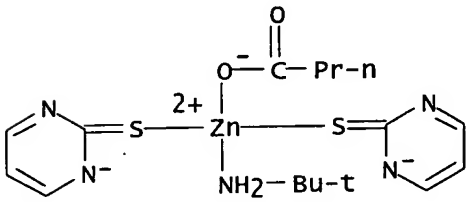

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1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE 1

AN 132:36842 CA
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AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
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CC 39-10 (Synthetic Elastomers and Natural Rubber)
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zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.

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IT Molecular structure-property relationship
Sulfidation
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Vulcanization accelerators and agents
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IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
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10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
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252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
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IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
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IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
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IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
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IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
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RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD

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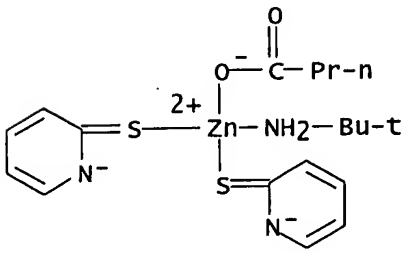
L9 ANSWER 37 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-36-6 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyridinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C18 H26 N3 O2 S2 Zn . H
CI CCS

SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (750557-81-4)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N	NC5	6	C5N	46.156.21	2



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RL: MOA (Modifier or additive use); USES (Uses)
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IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
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IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
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IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
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L9 ANSWER 38 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-35-5 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(2(1H)-pyrazinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
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LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)

CRN (740072-13-3)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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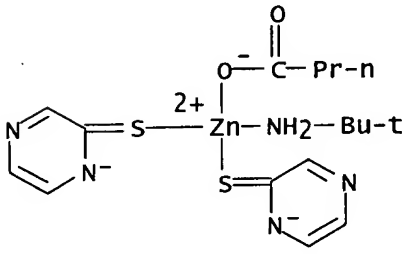

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L9 ANSWER 39 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-34-4 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4-nitro-2(1H)-pyridinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C18 H24 N5 O6 S2 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (774525-06-3)

Ring System Data

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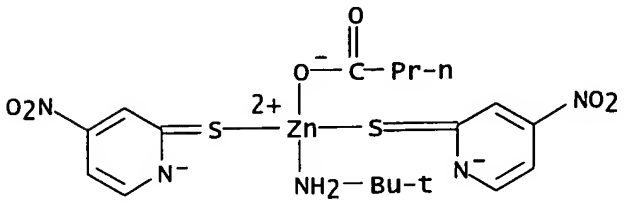

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1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)
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ST sulfur vulcanization SBR quant structure property relationship
IT Molecular structure-property relationship
Sulfidation
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IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)

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IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, Sulfur, uses
10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
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252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
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IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
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IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)

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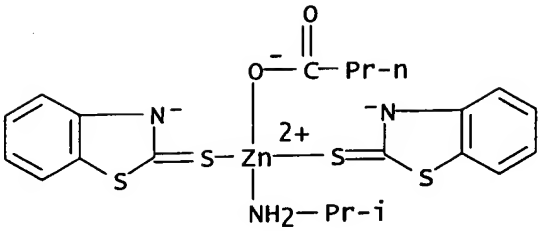
L9 ANSWER 40 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-31-1 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C21 H24 N3 O2 S4 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (765886-51-9)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



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IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
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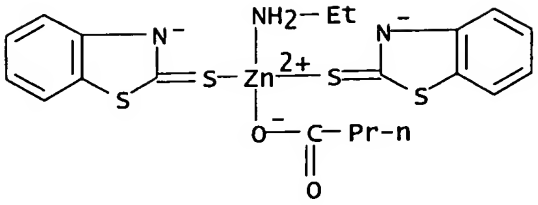
RN 252564-30-0 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(ethanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C20 H22 N3 O2 S4 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (760160-39-2)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



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252564-36-6 252564-37-7 252564-38-8 252564-83-3

RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)

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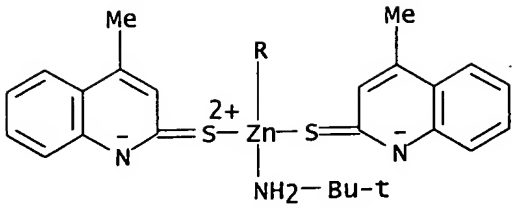
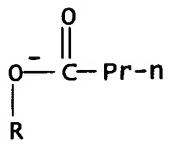
L9 ANSWER 42 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-28-6 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C28 H34 N3 O2 S2 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (755740-20-6)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C5N-C6	NC5-C6	6-6	C9N	591.79.43	2





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1 REFERENCES IN FILE CA (1907 TO DATE)
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REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)
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ST sulfur vulcanization SBR quant structure property relationship
IT Molecular structure-property relationship
Sulfidation
Vulcanization
Vulcanization accelerators and agents
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, sulfur, uses
10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
156017-14-0 156477-90-6 157993-40-3 188036-96-6 252564-20-8
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RL: MOA (Modifier or additive use); USES (Uses)
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IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
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IT 252564-18-4P
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IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
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L9 ANSWER 43 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-27-5 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zinc, bis(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C28 H38 N4 S2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)

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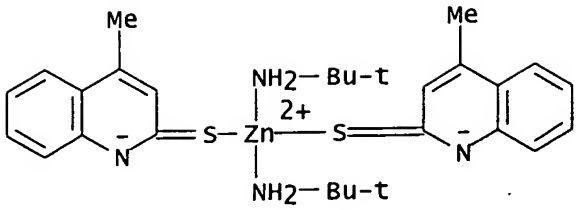

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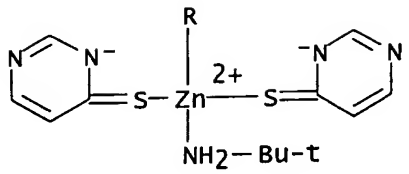
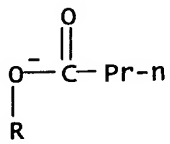
(66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS

L9 ANSWER 44 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-26-4 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zincate(1-), (butanoato-κO)(2-methyl-2-propanamine)bis(4(1H)-pyrimidinethionato-κS4)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 O2 S2 Zn . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
CRN (767616-38-6)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4N2	NCNC3	6	C4N2	46.195.23	2





1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)
AB Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
ST sulfur vulcanization SBR quant structure property relationship
IT Molecular structure-property relationship
Sulfidation
Vulcanization
Vulcanization accelerators and agents
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, Sulfur, uses

10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
156017-14-0 156477-90-6 157993-40-3 188036-96-6 252564-20-8
252564-21-9 252564-22-0 252564-23-1 252564-24-2 252564-25-3
252564-26-4 252564-27-5 252564-28-6 252564-29-7 252564-30-0
252564-31-1 252564-32-2 252564-33-3 252564-34-4 252564-35-5
252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS
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(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
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(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS
(61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS
(62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965, P53
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
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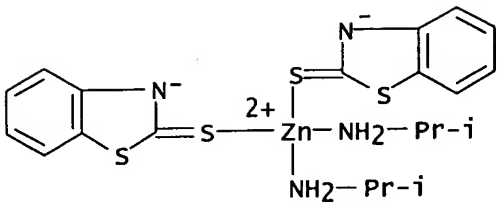
L9 ANSWER 45 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 252564-24-2 REGISTRY
ED Entered STN: 10 Jan 2000
CN Zinc, bis(2(3H)-benzothiazolethionato-κS2)bis(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C20 H26 N4 S4 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



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AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)
AB Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
ST sulfur vulcanization SBR quant structure property relationship
IT Molecular structure-property relationship
Sulfidation
Vulcanization
Vulcanization accelerators and agents
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, Sulfur, uses
10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
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252564-31-1 252564-32-2 252564-33-3 252564-34-4 252564-35-5
252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide

RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)

IT 9003-55-8
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)

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(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
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(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
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(41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS

(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
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(47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
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(50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
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(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
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(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS
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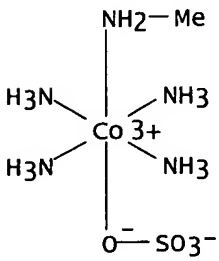
(63) Watson, A; PhD Thesis University of London 1965, P53
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
(65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS
(66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS

L9 ANSWER 46 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 210574-34-8 REGISTRY
ED Entered STN: 30 Aug 1998
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κO]-, (OC-6-23)-(9CI) (CA INDEX NAME)
MF C H17 Co N5 O4 S
CI CCS, COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent)



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 137:84151 CA
TI Activation volumes for a series of spontaneous, acid-and base-catalysed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-)

AU Benzo, Fabian; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz
CS Catedra de Quimica Inorganica, Facultad de Quimica, Universidad de la Republica, Montevideo, 11800, Urug.
SO Inorganic Reaction Mechanisms (Amsterdam, Netherlands) (2001), 3(1), 25-29
CODEN: IRMEFE; ISSN: 1028-6624
PB Gordon & Breach Science Publishers
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB The vols. of activation for the spontaneous, base-, and acid- catalyzed path of the hydrolysis reaction of a series of trans-[Co(MeNH2)(NH3)4X](3-n)+ ions (X = Cl-, Br-, (ONO2)- (OSO3)2-) have been determined in order to establish analogies with the dissociative trends found in previous work with the spontaneous hydrolysis of neutral ligands from the same cores. While for the base catalyzed path a significant decrease in the activation volume is found on going from the {Co(NH3)5} to the trans-{Co(MeNH2)(NH3)4} inert skeleton (i.e. 9.8, 12.5, 4.0 and 9.1 cm3mol-1 for the chloro, bromo, nitrato and sulfato derivs.), no significant changes are observed for the same complexes in the spontaneous reaction. The trends are rationalized in terms of the important changes occurring in electrostriction factors for the DCB and Id intimate mechanisms operating and the important increase in the degree of dissociativeness due to the presence of a trans-methylamino ligand. For the acid catalyzed path the differences are much more difficult to assess, specially taking into account the limited information available as well as the inherent errors involved in the rate constant determination
ST acid catalyzed aquation anionic cobalt complex activation vol; base catalyzed aquation anionic cobalt complex activation vol
IT Activation volume
Aquation
Aquation catalysts
Electrostriction
(activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-))
IT Acids, uses
Bases, uses
RL: CAT (Catalyst use); USES (Uses)
(activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-))
IT Transition metal complexes
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-))
IT 36527-86-3 134066-27-6 134066-30-1 210574-34-8
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-))
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
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REFERENCE 2

AN 133:49533 CA
TI Aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobalt(III) complex ion
AU Benzo, Fabian; Capparelli, Alberto L.; Martire, Daniel O.; Sienra, Beatriz
CS Catedra de Quimica Inorganica, Facultad de Quimica, Montevideo, C.C.1157, Urug.
SO Inorganic Reaction Mechanisms (Amsterdam) (2000), 1(4), 319-324
CODEN: IRMEFE; ISSN: 1028-6624
PB Gordon & Breach Science Publishers
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB The kinetics of aquation and base hydrolysis reactions of trans-[Co(NH3)4(NH2CH3)(OSO3)]+ have been studied. In acid solution the aquation rate, Raq, follows the equation Raq/[complex] = ks + kc[H+], at constant ionic strength μ = 1.0 M. The activation parameters are ΔHs# = 88.8 kJ mol-1, ΔSs# = -50.5 JK-1 mol-1, ΔHc# = 96.7 kJ mol-1 and ΔSc# = -23 JK-1 mol-1. The rate consts. at 25°C are ks = 4.15 + 10-6 s-1 and kc = 4.52 M-1 s-1. The rate of base hydrolysis, ROH, follows the equation ROH/[complex] = kOH [OH-]. The activation parameters are ΔHOH# = 74.9 kJmol-1 and ΔSOH# = 2JK-1 mol-1 and the rate constant is kOH = 0.58 M-1 s-1 at 25°C and μ = 0.15 M. The stereochem. of the hydroxo product has been determined (cis-[Co(NH3)4(NH2CH3)-(OH)]2+ = 9%). The results are discussed in the light of the reaction mechanisms proposed so far.
ST aquation kinetics mechanism ammine methylamine sulfato cobalt complex ion
IT Activation enthalpy
Activation entropy
Aquation kinetics
(aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobalt(III) complex ion)
IT Hydrolysis
(base, mechanism; aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobalt(III) complex ion)
IT Hydrolysis kinetics
(base; aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobalt(III) complex ion)
IT Aquation
(mechanism; aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobalt(III) complex ion)
IT 210574-34-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatoc
obalt(III) complex ion)

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CAPLUS

REFERENCE 3

AN 129:141178 CA
TI Competition study for the base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ complexes
AU Benzo, Fabian; Mendoza, Carolina; Queirolo, Marcelo; Sienra, Beatriz
CS Quimica Inorganica, Facultad de Quimica, Montevideo, Urug.
SO Polyhedron (1998), 17(13-14), 2295-2299
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB Nitrite ion competition has been measured for the base hydrolysis reaction of trans-Co(N-H3)4(NH2CH3)Xn+ ions (X = Cl-, Br-, NO3- and SO42-) in 1.0 M NaNO2 at 25°C. Both O- and N- bonded Co(NH3)4(NH2CH3)NO22+ are formed. Subsequently the Co(NH3)4(NH2CH3)ONO2+ isomer rearranges in OH- to give the thermodynamically more stable Co(NH3)4(NH2CH3)NO22+ ion. The total NO2- captured shows a slight dependence on the overall charge of the complex and on the nature of X (R = 2.2, 2.1, 3.6 and 1.2±0.5% for X = Cl-, Br-, NO3- and SO42-, resp.). These results differ from those observed

with complexes of the type Co(NH3)5Xn+ and Co(NH2CH3)5Xn+ where X includes a variety of anions.
ST base hydrolysis kinetics cobalt ammine complex
IT Hydrolysis
Hydrolysis kinetics
(base; competition study for base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ complexes)
IT 14797-65-0, Nitrite, reactions 36527-86-3 134066-27-6 134066-30-1 210574-34-8
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(competition study for base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ complexes)
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Balt, S; Trans Met Chem 1984, V9, P224 CAPLUS
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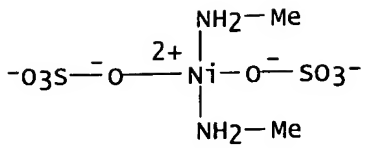
L9 ANSWER 47 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 202406-49-3 REGISTRY
ED Entered STN: 11 Mar 1998
CN Nickelate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, dihydrogen, hexahydrate (9CI) (CA INDEX NAME)
MF C2 H10 N2 Ni O8 S2 . 6 H2 O . 2 H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties)
CRN (791764-59-5)



●2 H^+

●6 H_2O

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 128:146849 CA
TI Infrared and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni
AU Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B.
CS Department of Physics, St. Gregorios College, Kottarakara, 691531, India
SO Journal of Solid State Chemistry (1997), 133(2), 407-415
CODEN: JSSCBI; ISSN: 0022-4596
PB Academic Press
DT Journal
LA English
CC 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
AB FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2·6H2O > (CH3NH3)2Ni (SO4)2·6H2O > (CH3NH3)2Zn(SO4)2·6H2O > Na2Cu(SO4)2·2H2O. The appearance of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and SO42- groups. The appearance of multiple bands in the bending and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mols. in (CH3NH3)2Cu(SO4)2·6H2O and (CH3NH3)2 Zn(SO4)2·6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2·6H2O.
ST IR Raman spectra metal sulfate hydrate; copper sodium sulfate dihydrate vibrational spectra; transition metal methylammonium sulfate hexahydrate; zinc methylammonium disulfate hexahydrate vibrational spectra; nickel methylammonium disulfate hexahydrate vibrational spectra
IT Hydrogen bond
(intramol.; in transition metal methylammonium sulfate hexahydrates studied with vibrational spectra)

IT IR spectra
Molecular vibration
Raman spectra
Vibrational spectra
(of copper sodium sulfate dihydrate and transition metal methylammonium sulfate hexahydrates)
IT Transition metal salts
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)
(vibrational spectra of copper, zinc, and nickel methylammonium sulfate hexahydrates)
IT 18901-72-9, Copper sodium sulfate (CuNa2(SO4)2) dihydrate 202406-41-5, Copper sodium sulfate (CuNa2(SO4)2) dideuterate
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)
(IR and Raman spectra and internal vibrational mode assignments)
IT 202406-44-8 202406-47-1 202406-49-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)
(IR and Raman spectra, internal vibrational mode assignments, and hydrogen bonding)
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
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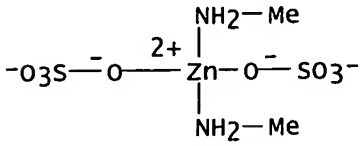
L9 ANSWER 48 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 202406-47-1 REGISTRY
ED Entered STN: 11 Mar 1998
CN Zincate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, dihydrogen, hexahydrate, (T-4)- (9CI) (CA INDEX NAME)

MF C2 H10 N2 O8 S2 Zn . 6 H2 O . 2 H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties)
CRN (745776-79-8)



●2 H^+

●6 H_2O

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 128:146849 CA
TI Infrared and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni
AU Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B.
CS Department of Physics, St. Gregorios College, Kottarakara, 691531, India
SO Journal of Solid State Chemistry (1997), 133(2), 407-415
CODEN: JSSCBI; ISSN: 0022-4596
PB Academic Press
DT Journal
LA English
CC 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
AB FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2·6H2O > (CH3NH3)2Ni (SO4)2·6H2O > (CH3NH3)2Zn(SO4)2·6H2O > Na2Cu(SO4)2·2H2O. The appearance of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and SO42- groups. The appearance of multiple bands in the bending and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mols. in

(CH3NH3)2Cu(SO4)2·6H2O and (CH3NH3)2 Zn(SO4)2·6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2·6H2O.

ST IR Raman spectra metal sulfate hydrate; copper sodium sulfate dihydrate vibrational spectra; transition metal methylammonium sulfate hexahydrate; zinc methylammonium disulfate hexahydrate vibrational spectra; nickel methylammonium disulfate hexahydrate vibrational spectra

IT Hydrogen bond
(intramol.; in transition metal methylammonium sulfate hexahydrates studied with vibrational spectra)

IT IR spectra
Molecular vibration
Raman spectra
Vibrational spectra
(of copper sodium sulfate dihydrate and transition metal methylammonium sulfate hexahydrates)

IT Transition metal salts
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(vibrational spectra of copper, zinc, and nickel methylammonium sulfate hexahydrates)

IT 18901-72-9, Copper sodium sulfate (CuNa2(SO4)2) dihydrate 202406-41-5, Copper sodium sulfate (CuNa2(SO4)2) dideuterate
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(IR and Raman spectra and internal vibrational mode assignments)

IT 202406-44-8 202406-47-1 202406-49-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(IR and Raman spectra, internal vibrational mode assignments, and hydrogen bonding)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

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(4) Bellanato, J; Spectrochim Acta 1960, V16, P1344 CAPLUS
(5) Campbell, J; Spectrochim Acta A 1970, V26, P2351 CAPLUS
(6) Dahlman, B; Ark Min 1952, V1, P339 CAPLUS
(7) Fateley, W; Infrared and Raman Selection Rules for Molecular and Lattice Vibrations - The Correlation Method 1972
(8) Gattow, G; Act Crystallogr 1958, V11, P377 CAPLUS
(9) Gattow, G; Acta Crystallogr 1958, V11, P866 CAPLUS
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(15) Jayakumar, V; Phys Status Solid 1988, V109, P635 CAPLUS
(16) Jordanovska, V; J Therm Anal 1992, V38, P1563 CAPLUS
(17) Kamoun, M; Spectrochim Acta A 1988, V44, P471
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(20) Mazzi, F; Acta Crystallogr 1955, V8, P137 CAPLUS
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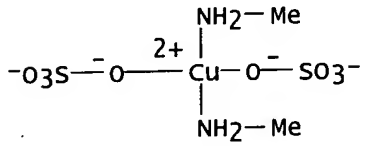
L9 ANSWER 49 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 202406-44-8 REGISTRY
ED Entered STN: 11 Mar 1998
CN Cuprate(2-), bis(methanamine)bis[sulfato(2-)-κO]-, dihydrogen, hexahydrate (9CI) (CA INDEX NAME)
MF C2 H10 Cu N2 O8 S2 . 6 H2 O . 2 H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties)
CRN (742042-77-9)



●2 H+

●6 H2O

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 128:146849 CA
TI Infrared and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni
AU Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B.
CS Department of Physics, St. Gregorios College, Kottarakara, 691531, India
SO Journal of Solid State Chemistry (1997), 133(2), 407-415
CODEN: JSSCBI; ISSN: 0022-4596
PB Academic Press
DT Journal
LA English
CC 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
AB FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2·6H2O > (CH3NH3)2Ni (SO4)2·6H2O > (CH3NH3)2Zn(SO4)2·6H2O > Na2Cu(SO4)2·2H2O. The appearance

of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and SO42- groups. The appearance of multiple bands in the bending and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mols. in (CH3NH3)2Cu(SO4)2·6H2O and (CH3NH3)2 Zn(SO4)2·6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2·6H2O.

ST IR Raman spectra metal sulfate hydrate; copper sodium sulfate dihydrate vibrational spectra; transition metal methylammonium sulfate hexahydrate; zinc methylammonium disulfate hexahydrate vibrational spectra; nickel methylammonium disulfate hexahydrate vibrational spectra

IT Hydrogen bond
(intramol.; in transition metal methylammonium sulfate hexahydrates studied with vibrational spectra)

IT IR spectra
Molecular vibration
Raman spectra
Vibrational spectra
(of copper sodium sulfate dihydrate and transition metal methylammonium sulfate hexahydrates)

IT Transition metal salts
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(vibrational spectra of copper, zinc, and nickel methylammonium sulfate hexahydrates)

IT 18901-72-9, Copper sodium sulfate (CuNa2(SO4)2) dihydrate 202406-41-5, Copper sodium sulfate (CuNa2(SO4)2) dideuterate
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(IR and Raman spectra and internal vibrational mode assignments)

IT 202406-44-8 202406-47-1 202406-49-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(IR and Raman spectra, internal vibrational mode assignments, and hydrogen bonding)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Abraham, S; J Raman Spectrosc 1991, V22, P245 CAPLUS
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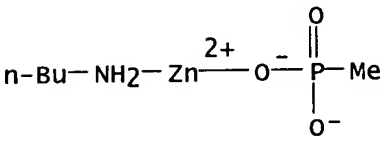
L9 ANSWER 50 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 184824-62-2 REGISTRY
ED Entered STN: 09 Jan 1997
CN Zinc, (1-butanamine)[methylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)
MF C5 H14 N O3 P Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:8432 CA
TI An organometallic route to zinc phosphonates and their intercalates
AU Gerbier, Philippe; Guerin, Christian; Henner, Bernard; Unal, Jean-Remi
CS U.M.R. 5637 -Universite Montpellier II, Montpellier, 34095, Fr.
SO Journal of Materials Chemistry (1999), 9(10), 2559-2565
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB An organometallic nonaq. route to zinc phosphonates and to their intercalates was studied. Various phosphonic acids react with dimethylzinc in THF media to afford the corresponding layered zinc phosphonates Zn(O3PR1) (R1 = Me, Ph, 2- and 3-thienyl, thiophen-3-ylmethyl) with evolution of methane. The presence of a primary n-alkylamine in the reaction mixture allows the 1-pot formation of 2-dimensional-layered intercalated phases Zn(O3PR1)·RNH2 [R2 = Bu, Penn (n-pentyl)] whereas a more bulky amine such as cyclohexylamine (HexcNH2) give 1-dimensional polymeric chains Zn(O3PPh)·2HexcNH2.
ST zinc phosphonate hydrate alkylamine intercalate prepn
IT Amines, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(aliphatic, zinc intercalate complexes; preparation of zinc phosphonate

alkylamine intercalation compds. from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectra)

IT NMR (nuclear magnetic resonance)
(phosphorus-31 CP MAS NMR spectra of zinc phosphonates and their hydrates and alkylamine intercalation compds., and relationship to phosphonate connectivity)

IT Intercalation compounds
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectra)

IT 108-91-8, Cyclohexanamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route)

IT 122-52-1, Triethylphosphite 544-97-8, Dimethylzinc 872-31-1, 3-Bromothiophene 993-13-5, Methylphosphonic acid 1003-09-4, 2-Bromothiophene 1571-33-1, Phenylphosphonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc phosphonates and their hydrates and alkylamine intercalation compds. from organometallic nonaq. route)

IT 13640-95-4P 21042-06-8P 113282-79-4P, 3-Thienylphosphonic acid 113305-47-8P, 2-Thienylphosphonic acid 188565-05-1P, Thiophen-3-ylmethylphosphonic acid 251323-56-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of zinc phosphonates and their hydrates and alkylamine intercalation compds. from organometallic nonaq. route)

IT 72702-22-8P, Zinc phenylphosphonate monohydrate 115320-62-2P, Zinc methylphosphonate monohydrate 251323-48-5P, Zinc 2-thienylphosphonate monohydrate 251323-49-6P, Zinc 3-thienylphosphonate monohydrate 251323-50-9P, Zinc thiophen-3-ylmethylphosphonate monohydrate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectrum)

IT 162050-26-2P 162050-27-3P 184824-62-2P 251323-51-0P 251323-52-1P 251323-53-2P 251323-54-3P 251323-55-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectrum of intercalate)

IT 133075-33-9P, Zinc methylphosphonate 251323-45-2P, Zinc 2-thienylphosphonate 251323-46-3P, Zinc 3-thienylphosphonate 251323-47-4P, Zinc thiophen-3-ylmethylphosphonate
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation from organometallic nonaq. route, interlayer spacing, 31P CP MAS NMR spectrum and hydration)

IT 34335-10-9P, Zinc phenylphosphonate
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation from organometallic nonaq. route, interlayer spacing, 31P CP MAS NMR spectrum, hydration and intercalation of alkylamines)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

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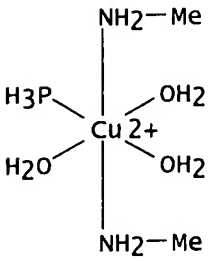
REFERENCE 2

AN 126:41873 CA
TI Structure of Zn(O3PC2H4CO2H)·0.5C6H5NH2 and XANES-EXAFS study of the intercalation of amines into Zn(O3PR)·H2O zinc alkylphosphonates
AU Drumel, Stephanie; Janvier, Pascal; Bujoli-Doeuff, Martine; Bujoli, Bruno
CS IMN, UMR CNRS 110, Faculte des Sciences et des Techniques, Nantes, 44072, Fr.
SO Journal of Materials Chemistry (1996), 6(11), 1843-1847
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
AB From XANES-EXAFS expts., neither the dehydration nor the subsequent n-alkylamine intercalation in Zn(O3PCH3)·H2O appears to be topotactic. On the contrary, the whole process consists of breaking Zn-O bonds present in the hydrated material, so that no bridging oxygen remains in the inorg. sheet. This hypothesis is supported by the structural determination of an aniline intercalate: Zn(O3PC2H4CO2H)·0.5C6H5NH2 [orthorhombic, space group Pbcn, a 29.880(6), b 8.526(2), c 14.720(3) Å, Z = 16, R = 0.043 and Rw = 0.047; 2063 observed reflections, I > 2σ(I)]. For steric reasons, only half of the zinc atoms are coordinated to aniline; the 2nd half of the metal atoms that are not bound to the amine retain the environment present in the initial anhydrous phase.
ST crystal structure zinc carboxyethylphosphonate aniline intercalated; zinc carboxyethylphosphonate aniline intercalated prepn structure; alkylphosphonate zinc alkylamine intercalation
IT EXAFS spectra
XANES spectra
(of zinc alkylphosphonates and their aqua or butylamine intercalation complexes)

IT Crystal structure
Molecular structure
(of zinc carboxyethylphosphonate aniline intercalation complex)
IT 133075-33-9 166671-21-2 184824-61-1 184824-62-2
RL: PRP (Properties)
(XANES-EXAFS spectra of)
IT 5962-42-5, 2-Carboxyethylphosphonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc carboxyethylphosphonate aniline intercalation complex)
IT 184824-60-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(polymeric; preparation and crystal structure of)

L9 ANSWER 51 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 182930-97-8 REGISTRY
ED Entered STN: 07 Nov 1996
CN Copper(2+), triaquabis(methanamine)(phosphine)-, (OC-6-22)- (9CI) (CA INDEX NAME)
MF C2 H19 Cu N2 O3 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PROC (Process); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 125:286037 CA
TI Quantum-chemical studies on the mechanism of the novel reaction of oxidative amination of P4 in the copper(II) coordination sphere
AU Dorfman, Ya. A.; Abdreimova, R. R.
CS Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy of Sciences of Kazakhstan, Almaty, Kazakhstan
SO Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
CODEN: RJCCEY; ISSN: 1070-3284
PB MAIK Nauka/Interperiodica
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 65
AB A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant.

formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II)→Cu(0) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra- and interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions.

ST mechanism oxidative amination phosphorus copper acidoamido; kinetics oxidative amination phosphorus copper acidoamido; quantum chem mechanism oxidative amination phosphorus

IT Kinetics of amination
(mechanism; quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT Amination
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

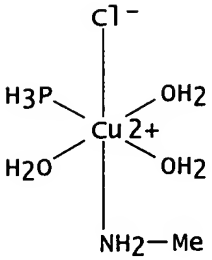
IT Molecular orbital
(CNDO, quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT 182930-77-4 182930-78-5 182930-79-6 182930-80-9 182930-81-0
182930-82-1 182930-83-2 182930-84-3 182930-85-4 182930-86-5
182930-87-6 182930-88-7 182930-89-8 182930-90-1 182930-91-2
182930-92-3 182930-93-4 182930-94-5 182930-95-6 182930-96-7
182930-97-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT 12185-10-3, Phosphorus(p4), reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

L9 ANSWER 52 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 182930-94-5 REGISTRY
ED Entered STN: 07 Nov 1996
CN Copper(1+), triaquachloro(methanamine)(phosphine)-, (OC-6-43)- (9CI) (CA INDEX NAME)
MF C H14 Cl Cu N O3 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PROC

(Process); PRP (Properties); RACT (Reactant or reagent)



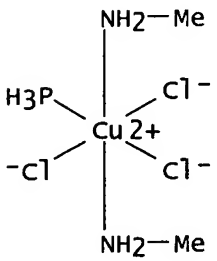
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 125:286037 CA
TI Quantum-chemical studies on the mechanism of the novel reaction of oxidative amination of P4 in the copper(II) coordination sphere
AU Dorfman, Ya. A.; Abdreimova, R. R.
CS Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy of Sciences of Kazakhstan, Almaty, Kazakhstan
SO Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
CODEN: RJCCEY; ISSN: 1070-3284
PB MAIK Nauka/Interperiodica
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 65
AB A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II)→Cu(0) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra- and interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions.
ST mechanism oxidative amination phosphorus copper acidoamido; kinetics oxidative amination phosphorus copper acidoamido; quantum chem mechanism oxidative amination phosphorus

IT Kinetics of amination
(mechanism; quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)
IT Amination
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)
IT Molecular orbital
(CNDO, quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)
IT 182930-77-4 182930-78-5 182930-79-6 182930-80-9 182930-81-0
182930-82-1 182930-83-2 182930-84-3 182930-85-4 182930-86-5
182930-87-6 182930-88-7 182930-89-8 182930-90-1 182930-91-2
182930-92-3 182930-93-4 182930-94-5 182930-95-6 182930-96-7
182930-97-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)
IT 12185-10-3, Phosphorus(p4), reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

L9 ANSWER 53 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 182930-88-7 REGISTRY
ED Entered STN: 07 Nov 1996
CN Cuprate(1-), trichlorobis(methanamine)(phosphine)-, (OC-6-21)- (9CI) (CA INDEX NAME)
MF C2 H13 Cl3 Cu N2 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents.: FORM (Formation, nonpreparative); PROC (Process); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 125:286037 CA
TI Quantum-chemical studies on the mechanism of the novel reaction of oxidative amination of P4 in the copper(II) coordination sphere
AU Dorfman, Ya. A.; Abdreimova, R. R.
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of Sciences of Kazakhstan, Almaty, Kazakhstan
SO Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
CODEN: RJCCEY; ISSN: 1070-3284
PB MAIK Nauka/Interperiodica
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 65

AB A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II)→Cu(0) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra- and interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions.

ST mechanism oxidative amination phosphorus copper acidoamido; kinetics oxidative amination phosphorus copper acidoamido; quantum chem mechanism oxidative amination phosphorus

IT Kinetics of amination
(mechanism; quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

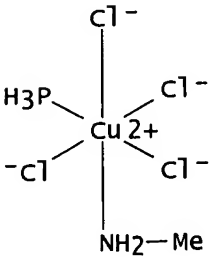
IT Amination
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT Molecular orbital
(CNDO, quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT 182930-77-4 182930-78-5 182930-79-6 182930-80-9 182930-81-0
182930-82-1 182930-83-2 182930-84-3 182930-85-4 182930-86-5
182930-87-6 182930-88-7 182930-89-8 182930-90-1 182930-91-2
182930-92-3 182930-93-4 182930-94-5 182930-95-6 182930-96-7
182930-97-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT 12185-10-3, Phosphorus(p4), reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

L9 ANSWER 54 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 182930-87-6 REGISTRY
ED Entered STN: 07 Nov 1996
CN Cuprate(2-), tetrachloro(methanamine)(phosphine)-, (OC-6-32)- (9CI) (CA INDEX NAME)
MF C H8 Cl4 Cu N P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PROC (Process); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 125:286037 CA
TI Quantum-chemical studies on the mechanism of the novel reaction of oxidative amination of P4 in the copper(II) coordination sphere
AU Dorfman, Ya. A.; Abdreimova, R. R.
CS Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy of Sciences of Kazakhstan, Almaty, Kazakhstan
SO Russian Journal of Coordination Chemistry (Translation of Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
CODEN: RJCCEY; ISSN: 1070-3284
PB MAIK Nauka/Interperiodica
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 65
AB A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the

two-electron Cu(II)→Cu(0) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra- and interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions.

ST mechanism oxidative amination phosphorus copper acidoamido; kinetics oxidative amination phosphorus copper acidoamido; quantum chem mechanism oxidative amination phosphorus

IT Kinetics of amination
(mechanism; quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

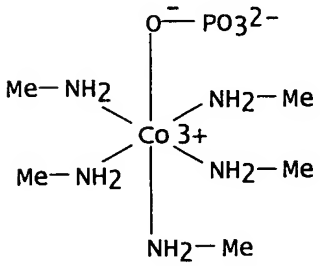
IT Amination
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT Molecular orbital
(CNDO, quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT 182930-77-4 182930-78-5 182930-79-6 182930-80-9 182930-81-0
182930-82-1 182930-83-2 182930-84-3 182930-85-4 182930-86-5
182930-87-6 182930-88-7 182930-89-8 182930-90-1 182930-91-2
182930-92-3 182930-93-4 182930-94-5 182930-95-6 182930-96-7
182930-97-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

IT 12185-10-3, Phosphorus(p4), reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)

L9 ANSWER 55 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 173178-23-9 REGISTRY
ED Entered STN: 13 Feb 1996
CN Cobalt, pentakis(methanamine)[phosphato(3-)-O]-, (OC-6-22)- (9CI) (CA INDEX NAME)
MF C5 H25 Co N5 O4 P
CI CCS, COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent)



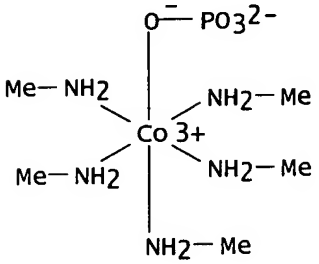
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 124:128031 CA
TI Outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes. A temperature- and pressure-dependence kinetic study on the effects of the different {N5} groups
AU Martinez, Manuel; Pitarque, Mari-Angel
CS Facultat Quimica, Universitat Barcelona, Barcelona, E-08028, Spain
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (24), 4107-11
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 69, 78
AB Outer-sphere redox reactions between [Co{N5}(HnPO4)]n+[{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane (L)] and [Fe(CN)6]4- have been studied as a function of pH, {N5}, temperature and pressure. The effect of the size of the {N5} skeleton, has been investigated for the n = 0, 1, 2 systems in order to establish possible correlations between the size and charge of the cobalt(III) complex and the ion-pair formation constant, the electron-transfer rate constant, and the thermal and baric activation parameters. The values obtained indicate that the ion-pair formation consts. are the same, within exptl. error, for all the systems studied. The electron-transfer rate constant for a given degree (n = 1) of protonation of the [Co{N5}(HnPO4)]n+ complex increases on increasing the size of the monodentate amines, while an important decrease is observed when they are substituted by the N5 macrocycle (L) [2.6 + 10-3 s-1, {N5} = (NH3)5, 59 + 10-3 s-1, {N5} = (NH2Me)5, 0.73 + 10-3 s-1, {N5} = L; resp. at 35°C]. The activation enthalpies do not show any significant change, neither with decreasing charge on the cobalt complex nor with the size of the amine. The values of ΔS.thermod. and ΔV.thermod. vary considerably with the degree of protonation of the phosphate ligands and the size of the CoIII cavity of the complexes. The opposite trends observed for the values of ΔS.thermod. [8 J K-1 mol-1 for {N5} = (NH2Me)5 (n = 1); -61 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 32 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 17 cm3 mol-1 for {N5} = (NH3)5 (n = 0)] are related to the existence of an important increase in hydrogen bond formation in the cobalt(III) complex on going to the transition state.
ST cobalt macrocycle complex redox reaction kinetics
IT Electron exchange and Charge transfer
Protonation and Proton transfer reaction
Redox reaction
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes)
IT Hydrogen bond
Ion pairs
Kinetics of electron exchange
Kinetics of protonation
Kinetics of redox reaction
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes and temperature- and pressure-dependence kinetic effects of different {N5})

IT 13408-63-4 15612-03-0 19169-72-3 19306-79-7 173178-22-8
173178-23-9 173178-24-0
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes and temperature- and pressure-dependence kinetic effects of different {N5})

L9 ANSWER 56 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 173178-22-8 REGISTRY
ED Entered STN: 13 Feb 1996
CN Cobalt, pentakis(methanamine)[phosphato(3-)-O]-, conjugate monoacid, (OC-6-22)- (9CI) (CA INDEX NAME)
MF C5 H25 Co N5 O4 P . H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent)
CRN (173178-23-9)



● H+

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 124:128031 CA
TI Outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes. A temperature- and pressure-dependence kinetic study on the effects of the different {N5} groups
AU Martinez, Manuel; Pitarque, Mari-Angel
CS Facultat Quimica, Universitat Barcelona, Barcelona, E-08028, Spain
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1995), (24), 4107-11
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 69, 78

AB Outer-sphere redox reactions between [Co{N5}(HnPO4)]n+[{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane (L)] and [Fe(CN)6]4- have been studied as a function of pH, {N5}, temperature and pressure. The effect of the size of the {N5} skeleton, has been investigated for the n = 0, 1, 2 systems in order to establish possible correlations between the size and charge of the cobalt(III) complex and the ion-pair formation constant, the electron-transfer rate constant, and the thermal and baric activation parameters. The values obtained indicate that the ion-pair formation consts. are the same, within exptl. error, for all the systems studied. The electron-transfer rate constant for a given degree (n = 1) of protonation of the [Co{N5}(HnPO4)]n+ complex increases on increasing the size of the monodentate amines, while an important decrease is observed when they are substituted by the N5 macrocycle (L) [2.6 + 10-3 s-1, {N5} = (NH3)5, 59 + 10-3 s-1, {N5} = (NH2Me)5, 0.73 + 10-3 s-1, {N5} = L; resp. at 35°C]. The activation enthalpies do not show any significant change, neither with decreasing charge on the cobalt complex nor with the size of the amine. The values of ΔS.thermod. and ΔV.thermod. vary considerably with the degree of protonation of the phosphate ligands and the size of the CoIII cavity of the complexes. The opposite trends observed for the values of ΔS.thermod. [8 J K-1 mol-1 for {N5} = (NH2Me)5 (n = 1); -61 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 32 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 17 cm3 mol-1 for {N5} = (NH3)5 (n = 0)] are related to the existence of an important increase in hydrogen bond formation in the cobalt(III) complex on going to the transition state.

ST cobalt macrocycle complex redox reaction kinetics

IT Electron exchange and Charge transfer
Protonation and Proton transfer reaction
Redox reaction
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes)

IT Hydrogen bond
Ion pairs
Kinetics of electron exchange
Kinetics of protonation
Kinetics of redox reaction
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes and temperature- and pressure-dependence kinetic effects of different {N5})

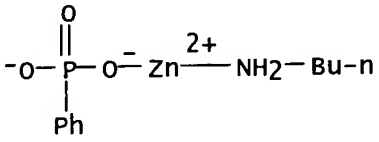
IT 13408-63-4 15612-03-0 19169-72-3 19306-79-7 173178-22-8 173178-23-9 173178-24-0
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes and temperature- and pressure-dependence kinetic effects of different {N5})

L9 ANSWER 57 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 162050-26-2 REGISTRY
ED Entered STN: 07 Apr 1995
CN Zinc, (1-butanamine)[phenylphosphonato(2-)-κO]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Zinc, (1-butanamine)[phenylphosphonato(2-)-O]-
MF C10 H16 N O3 P Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:8432 CA
TI An organometallic route to zinc phosphonates and their intercalates
AU Gerbier, Philippe; Guerin, Christian; Henner, Bernard; Unal, Jean-Remi
CS U.M.R. 5637 -Universite Montpellier II, Montpellier, 34095, Fr.
SO Journal of Materials Chemistry (1999), 9(10), 2559-2565
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB An organometallic nonaq. route to zinc phosphonates and to their intercalates was studied. Various phosphonic acids react with dimethylzinc in THF media to afford the corresponding layered zinc phosphonates Zn(O3PR1) (R1 = Me, Ph, 2- and 3-thienyl, thiophen-3-ylmethyl) with evolution of methane. The presence of a primary n-alkylamine in the reaction mixture allows the 1-pot formation of 2-dimensional-layered intercalated phases Zn(O3PR1)·RNH2 [R2 = Bu, Penn (n-pentyl)] whereas a more bulky amine such as cyclohexylamine (HexcNH2) give 1-dimensional polymeric chains Zn(O3PPh)·2HexcNH2.
ST zinc phosphonate hydrate alkylamine intercalate prepn
IT Amines, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(aliphatic, zinc intercalate complexes; preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectra)
IT NMR (nuclear magnetic resonance)
(phosphorus-31 CP MAS NMR spectra of zinc phosphonates and their hydrates and alkylamine intercalation compds., and relationship to phosphonate connectivity)
IT Intercalation compounds
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectra)
IT 108-91-8, Cyclohexanamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine

RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route)

IT 122-52-1, Triethylphosphite 544-97-8, Dimethylzinc 872-31-1, 3-Bromothiophene 993-13-5, Methylphosphonic acid 1003-09-4, 2-Bromothiophene 1571-33-1, Phenylphosphonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc phosphonates and their hydrates and alkylamine intercalation compds. from organometallic nonaq. route)

IT 13640-95-4P 21042-06-8P 113282-79-4P, 3-Thienylphosphonic acid 113305-47-8P, 2-Thienylphosphonic acid 188565-05-1P, Thiophen-3-ylmethylphosphonic acid 251323-56-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of zinc phosphonates and their hydrates and alkylamine intercalation compds. from organometallic nonaq. route)

IT 72702-22-8P, Zinc phenylphosphonate monohydrate 115320-62-2P, Zinc methylphosphonate monohydrate 251323-48-5P, Zinc 2-thienylphosphonate monohydrate 251323-49-6P, Zinc 3-thienylphosphonate monohydrate 251323-50-9P, Zinc thiophen-3-ylmethylphosphonate monohydrate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectrum)

IT 162050-26-2P 162050-27-3P 184824-62-2P 251323-51-0P 251323-52-1P 251323-53-2P 251323-54-3P 251323-55-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR spectrum of intercalate)

IT 133075-33-9P, Zinc methylphosphonate 251323-45-2P, Zinc 2-thienylphosphonate 251323-46-3P, Zinc 3-thienylphosphonate 251323-47-4P, Zinc thiophen-3-ylmethylphosphonate
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation from organometallic nonaq. route, interlayer spacing, 31P CP MAS NMR spectrum and hydration)

IT 34335-10-9P, Zinc phenylphosphonate
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation from organometallic nonaq. route, interlayer spacing, 31P CP MAS NMR spectrum, hydration and intercalation of alkylamines)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD

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REFERENCE 2

AN 124:67877 CA
TI Coordinative intercalation of alkylamines into layered zinc phenylphosphonate. Crystal structures from x-ray powder diffraction data
AU Poojary, Damodara M.; Clearfield, Abraham
CS Department of Chemistry, Texas AM University, College Station, TX, 77843, USA
SO Journal of the American Chemical Society (1995), 117(45), 11278-84
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 75, 78
AB Zn phenylphosphonate monohydrate takes up 1 mol of amine when contacted with liquid primary alkylamines. The mechanism of intercalation involves replacement of the coordinated H2O mol. by the amine mols. Although the composition of the intercalate Zn(O3PPh)(RNH2) is consistent with the anal. and spectroscopic data, there exist discrepancies in the observed interlayer d spacings of the intercalate with respect to that in the host compound The d spacing for the propylamine intercalate is in fact smaller than that in Zn phenylphosphonate itself. To understand this feature specifically and to explain the mechanism of amine intercalation in metal phosphonates in general, the authors determined the structures of the intercalates. The structures of Zn(O3PPh)(RNH2), R = -C3H9 (1), -C4H11 (2), -C5H13 (3), were solved ab initio from x-ray powder diffraction data and refined by Rietveld methods. All the compds. are isostructural, and they crystallize in the monoclinic space group P21/c with a 13.978(3), b 8.791(2), c 9.691(2) Å, and β 102.08(1)° for 1, a 14.698(4), b 8.957(3), c 9.712(3) Å, and β 102.465(3)° for 2, and a 16.267(3), b 8.935(2), c 9.695(2) Å, and β 102.32(1)° for 3. The structures of these intercalates are new and are different from that of the host compound although all of them are layered. In the intercalate the Zn atoms are tetrahedrally coordinated as opposed to octahedral coordination in the host compound
ST coordinative intercalation alkylamine zinc phenylphosphonate structure; intercalation coordinative alkylamine zinc phenylphosphonate structure
IT Inclusion reaction
(intercalation, of zinc phenylphosphonate monohydrate by alkylamines)
IT 107-10-8, Propylamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine 72702-22-8
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(coordinative intercalation of alkylamines into layered zinc phenylphosphonate and crystal structures from x-ray powder diffraction data)
IT 162050-25-1P 162050-26-2P 162050-27-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and crystal structure of)

REFERENCE 3

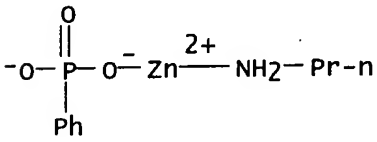
AN 122:229146 CA
TI Intercalation of alkylamines into dehydrated and hydrated zinc phenylphosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Department of Chemistry, Texas A and M Univ., College Station, TX, 77843, USA
SO Journal of Materials Chemistry (1995), 5(2), 315-18
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB Primary amines, CnH2n+1NH2 (n = 3-8), were intercalated into layered anhydrous Zn phenylphosphonate Zn(O3PPh) and its monohydrate Zn(O3PPh).H2O when the host compds. were brought into contact with liquid amines. In both cases, 1 mol of amine was intercalated forming layered compds. Zn(O3PPh).(RNH2) as characterized by powder x-ray diffraction, TG and IR spectroscopy. The amines coordinate to the Zn atoms at the site vacated by the H2O mol. A plot of the interlayer distances of the intercalates vs. the number of C atoms in the alkyl chain of the amine gives a straight line with a slope of 1.24 Å, which indicates that the alkyl chains are most likely packed as an interdigitated monolayer with a tilt angle of 78° with respect to the mean plane of the layer. A comparison of the intercalation reactions of Zn, Co and Cu Me- and phenyl-phosphonates is included in the discussion section.
ST intercalation alkylamine dehydrated hydrated zinc phenylphosphonate; amine alkyl intercalation zinc phenylphosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation of dehydrated and hydrated zinc phenylphosphonates by)
IT Molecular orientation
(of amines in amine intercalated zinc phenylphosphonates)
IT Inclusion reaction
(intercalation, of alkylamines with dehydrated and hydrated zinc phenylphosphonates)
IT 34335-10-9, Phosphonic acid, phenyl-, zinc salt (1:1) 72702-22-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation reaction with alkylamines)
IT 96-15-1, 2-Methylbutylamine 107-10-8, Propylamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine 111-26-2, Hexylamine 111-68-2, Heptylamine 111-86-4, Octylamine 112-20-9, Nonylamine 123-82-0, 2-Aminoheptane
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation reaction with dehydrated and hydrated phenylphosphonate)
IT 162050-25-1P 162050-26-2P 162050-27-3P 162050-28-4P 162050-29-5P 162050-30-8P 162050-31-9P 162050-32-0P 162050-33-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 58 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 162050-25-1 REGISTRY
ED Entered STN: 07 Apr 1995
CN Zinc, [phenylphosphonato(2-)-O](1-propanamine)- (9CI) (CA INDEX NAME)
MF C9 H14 N O3 P Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 124:67877 CA
TI Coordinative intercalation of alkylamines into layered zinc phenylphosphonate. Crystal structures from x-ray powder diffraction data
AU Poojary, Damodara M.; Clearfield, Abraham
CS Department of Chemistry, Texas AM University, College Station, TX, 77843, USA
SO Journal of the American Chemical Society (1995), 117(45), 11278-84
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 75, 78
AB Zn phenylphosphonate monohydrate takes up 1 mol of amine when contacted with liquid primary alkylamines. The mechanism of intercalation involves replacement of the coordinated H2O mol. by the amine mols. Although the composition of the intercalate Zn(O3PPh)(RNH2) is consistent with the anal. and spectroscopic data, there exist discrepancies in the observed interlayer d spacings of the intercalate with respect to that in the host compound The d spacing for the propylamine intercalate is in fact smaller than that in Zn phenylphosphonate itself. To understand this feature specifically and to explain the mechanism of amine intercalation in metal phosphonates in general, the authors determined the structures of the intercalates. The structures of Zn(O3PPh)(RNH2), R = -C3H9 (1), -C4H11 (2), -C5H13 (3), were solved ab initio from x-ray powder diffraction data and refined by Rietveld methods. All the compds. are isostructural, and they crystallize in the monoclinic space group P21/c with a 13.978(3), b 8.791(2), c 9.691(2) Å, and β 102.08(1)° for 1, a 14.698(4), b 8.957(3), c 9.712(3) Å, and β 102.465(3)° for 2, and a 16.267(3), b 8.935(2), c 9.695(2) Å, and β 102.32(1)° for 3. The structures of these intercalates are new and are different from that of the host compound although all of them are layered. In the intercalate the Zn atoms are tetrahedrally coordinated as opposed to octahedral coordination in the host compound
ST coordinative intercalation alkylamine zinc phenylphosphonate structure; intercalation coordinative alkylamine zinc phenylphosphonate structure

IT Inclusion reaction
(intercalation, of zinc phenylphosphonate monohydrate by alkylamines)
IT 107-10-8, Propylamine, reactions 109-73-9, Butylamine, reactions
110-58-7, Pentylamine 72702-22-8
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(coordinative intercalation of alkylamines into layered zinc phenylphosphonate and crystal structures from x-ray powder diffraction data)
IT 162050-25-1P 162050-26-2P 162050-27-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

REFERENCE 2

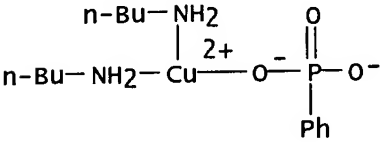
AN 122:229146 CA
TI Intercalation of alkylamines into dehydrated and hydrated zinc phenylphosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Department of Chemistry, Texas A and M Univ., College Station, TX, 77843, USA
SO Journal of Materials Chemistry (1995), 5(2), 315-18
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry
DT Journal
LA English
CC 78-3 (Inorganic Chemicals and Reactions)
AB Primary amines, CnH2n+1NH2 (n = 3-8), were intercalated into layered anhydrous Zn phenylphosphonate Zn(O3PPh) and its monohydrate Zn(O3PPh).H2O when the host compds. were brought into contact with liquid amines. In both cases, 1 mol of amine was intercalated forming layered compds. Zn(O3PPh).(RNH2) as characterized by powder x-ray diffraction, TG and IR spectroscopy. The amines coordinate to the Zn atoms at the site vacated by the H2O mol. A plot of the interlayer distances of the intercalates vs. the number of C atoms in the alkyl chain of the amine gives a straight line with a slope of 1.24 Å, which indicates that the alkyl chains are most likely packed as an interdigitated monolayer with a tilt angle of 78° with respect to the mean plane of the layer. A comparison of the intercalation reactions of Zn, Co and Cu Me- and phenyl-phosphonates is included in the discussion section.
ST intercalation alkylamine dehydrated hydrated zinc phenylphosphonate; amine alkyl intercalation zinc phenylphosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation of dehydrated and hydrated zinc phenylphosphonates by)
IT Molecular orientation
(of amines in amine intercalated zinc phenylphosphonates)
IT Inclusion reaction
(intercalation, of alkylamines with dehydrated and hydrated zinc phenylphosphonates)
IT 34335-10-9, Phosphonic acid, phenyl-, zinc salt (1:1) 72702-22-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation reaction with alkylamines)
IT 96-15-1, 2-Methylbutylamine 107-10-8, Propylamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine 111-26-2, Hexylamine 111-68-2, Heptylamine 111-86-4, Octylamine 112-20-9, Nonylamine 123-82-0, 2-Aminoheptane
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation reaction with dehydrated and hydrated phenylphosphonate)
IT 162050-25-1P 162050-26-2P 162050-27-3P 162050-28-4P 162050-29-5P 162050-30-8P 162050-31-9P 162050-32-0P 162050-33-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

L9 ANSWER 59 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 147578-80-1 REGISTRY
ED Entered STN: 14 May 1993
CN Copper, bis(1-butanamine)[phenylphosphonato-O]- (9CI) (CA INDEX NAME)
MF C14 H27 Cu N2 O3 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

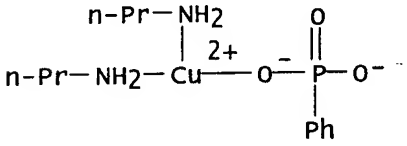
AN 118:234154 CA
TI Intercalation of alkylamines into layered copper phosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Chemistry of Materials (1993), 5(4), 495-9
CODEN: CMATEX; ISSN: 0897-4756
DT Journal
LA English
CC 29-7 (Organometallic and Organometalloidal Compounds)
AB Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3)·(RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates.
ST intercalation alkylamine layered dehydrated copper phosphonate; inclusion reaction alkylamine layered copper phosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl, intercalation of, into layered copper phosphonates)

IT Inclusion reaction
(intercalation, of alkylamines into layered copper phosphonates)
IT 107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine
109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 111-26-2P,
Hexylamine 111-68-2P, 1-Heptanamine 111-86-4P, Octylamine
RL: PREP (Preparation)
(intercalation of, into layered copper phosphonates)
IT 45986-30-9 71803-57-1 147578-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(interlayer spacing and dehydration of)
IT 141848-52-4P 147578-74-3P 147578-75-4P 147578-76-5P 147578-77-6P
147578-78-7P 147578-79-8P 147578-80-1P 147578-81-2P 147578-82-3P
147607-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer distances of)
IT 126013-69-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer spacing of)
IT 34001-96-2P 34335-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, interlayer spacing and intercalation of alkylamines into)

L9 ANSWER 60 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 147578-79-8 REGISTRY
ED Entered STN: 14 May 1993
CN Copper, [phenylphosphonato(2-)-O]bis(1-propanamine)- (9CI) (CA INDEX NAME)
MF C12 H23 Cu N2 O3 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1



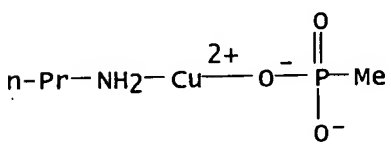
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 118:234154 CA
TI Intercalation of alkylamines into layered copper phosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Chemistry of Materials (1993), 5(4), 495-9

CODEN: CMATEX; ISSN: 0897-4756
DT Journal
LA English
CC 29-7 (Organometallic and Organometalloidal Compounds)
AB Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3)·(RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates.
ST intercalation alkylamine layered dehydrated copper phosphonate; inclusion reaction alkylamine layered copper phosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl, intercalation of, into layered copper phosphonates)
IT Inclusion reaction
(intercalation, of alkylamines into layered copper phosphonates)
IT 107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 111-26-2P, Hexylamine 111-68-2P, 1-Heptanamine 111-86-4P, Octylamine
RL: PREP (Preparation)
(intercalation of, into layered copper phosphonates)
IT 45986-30-9 71803-57-1 147578-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(interlayer spacing and dehydration of)
IT 141848-52-4P 147578-74-3P 147578-75-4P 147578-76-5P 147578-77-6P 147578-78-7P 147578-79-8P 147578-80-1P 147578-81-2P 147578-82-3P 147607-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer distances of)
IT 126013-69-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer spacing of)
IT 34001-96-2P, 34335-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, interlayer spacing and intercalation of alkylamines into)

L9 ANSWER 61 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 147578-74-3 REGISTRY
ED Entered STN: 14 May 1993
CN Copper, [methylphosphonato(2-)-O](1-propanamine)- (9CI) (CA INDEX NAME)
MF C4 H12 Cu N O3 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



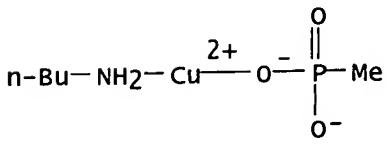
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 118:234154 CA
TI Intercalation of alkylamines into layered copper phosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Chemistry of Materials (1993), 5(4), 495-9
CODEN: CMATEX; ISSN: 0897-4756
DT Journal
LA English
CC 29-7 (Organometallic and Organometalloidal Compounds)
AB Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3)·(RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates.
ST intercalation alkylamine layered dehydrated copper phosphonate; inclusion reaction alkylamine layered copper phosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl, intercalation of, into layered copper phosphonates)
IT Inclusion reaction
(intercalation, of alkylamines into layered copper phosphonates)
IT 107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 111-26-2P, Hexylamine 111-68-2P, 1-Heptanamine 111-86-4P, Octylamine
RL: PREP (Preparation)
(intercalation of, into layered copper phosphonates)
IT 45986-30-9 71803-57-1 147578-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(interlayer spacing and dehydration of)
IT 141848-52-4P 147578-74-3P 147578-75-4P 147578-76-5P 147578-77-6P 147578-78-7P 147578-79-8P 147578-80-1P 147578-81-2P 147578-82-3P 147607-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer distances of)
IT 126013-69-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer spacing of)
IT 34001-96-2P 34335-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, interlayer spacing and intercalation of alkylamines into)

L9 ANSWER 62 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 141848-52-4 REGISTRY
ED Entered STN: 19 Jun 1992
CN Copper, (1-butanamine)[methylphosphonato(2-)-O]- (9CI) (CA INDEX NAME)
MF C5 H14 Cu N O3 P
CI CCS
SR CA
LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 118:234154 CA
TI Intercalation of alkylamines into layered copper phosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Chemistry of Materials (1993), 5(4), 495-9
CODEN: CMATEX; ISSN: 0897-4756
DT Journal
LA English
CC 29-7 (Organometallic and Organometalloidal Compounds)
AB Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3)·(RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates.
ST intercalation alkylamine layered dehydrated copper phosphonate; inclusion reaction alkylamine layered copper phosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl, intercalation of, into layered copper phosphonates)
IT Inclusion reaction
(intercalation, of alkylamines into layered copper phosphonates)
IT 107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 111-26-2P, Hexylamine 111-68-2P, 1-Heptanamine 111-86-4P, Octylamine
RL: PREP (Preparation)
(intercalation of, into layered copper phosphonates)
IT 45986-30-9 71803-57-1 147578-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(interlayer spacing and dehydration of)
IT 141848-52-4P 147578-74-3P 147578-75-4P 147578-76-5P 147578-77-6P 147578-78-7P 147578-79-8P 147578-80-1P 147578-81-2P 147578-82-3P 147607-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer distances of)
IT 126013-69-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer spacing of)
IT 34001-96-2P 34335-09-6P

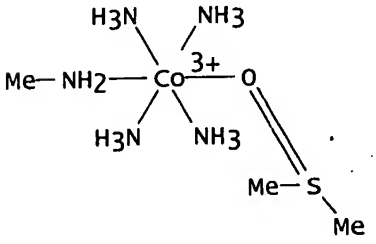
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, interlayer spacing and intercalation of alkylamines into)

REFERENCE 2

AN 117:19105 CA
TI Synthesis, crystal structures, and coordination intercalation behavior of two copper phosphonates
AU Zhang, Yiping; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Inorganic Chemistry (1992), 31(13), 2821-6
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
CC 78-5 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
AB Cu(O3PMe).H2O and Cu(O3PPh).H2O were synthesized and their structures determined Cu(O3PMe).H2O is monoclinic: space group P21/c, a 8.495(4), b 7.580(4), c 7.289(4) Å, β 90.08 (4)°, Z = 4, R = 0.030, Rw = 0.041. The structure is layered as formed by unusual 5-coordinate distorted tetragonal pyramidal Cu atoms. One O of each phosphonate bonds to 2 Cu atoms forming a chain, while the other 2 phosphonate O atoms bond to 2 Cu atoms in an adjacent chain. The base of the pyramid consists of 3 phosphonate O atoms and the coordinated H2O mol. All H bonds are of the intralayer type, so only van der Waals forces exist between adjacent layers. Amines are coordinatively intercalated with layer expansion. Cu(O3PPh).H2O is orthorhombic: space group Pbca, a 7.5547(4), b 7.4478(6), c 27.928(1) Å, Z = 8, R = 0.037 and Rw = 0.043. The coordination about the Cu atoms and the layer structure are identical to those of the O3PMe compound The Ph rings in the interlamellar space are oriented at a 98° angle to each other in adjacent rows. These structures are compared to those of other layered divalent phosphonates and Cu phosphites.
ST crystal structure copper phosphonate; amine intercalation copper phosphonate
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation of, in anhydrous and hydrous copper phosphonate)
IT Crystal structure
Molecular structure
(of copper phosphonate hydrates)
IT Inclusion reaction
(intercalation, of amine in anhydrous and hydrous copper phosphonate)
IT 109-73-9, Butylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(intercalation of, in anhydrous and hydrous copper phosphonate)
IT 71803-57-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure and intercalation reaction of, with amine)
IT 72702-21-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT 141848-52-4P 141848-53-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and interlayer spacing of intercalation compound)
IT 993-13-5, Methylphosphonic acid 1571-33-1, Phenylphosphonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cupric sulfate in presence of hydrolyzing urea)
IT 7758-98-7, Cupric sulfate, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with phosphonic acids in presence of hydrolyzing urea)

L9 ANSWER 63 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 138521-45-6 REGISTRY
ED Entered STN: 24 Jan 1992
CN Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-O]-, tribromide, (OC-6-23)- (9CI) (CA INDEX NAME)
MF C3 H23 Co N5 O S . 3 Br
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
CRN (138521-43-4)



●3 Br⁻

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

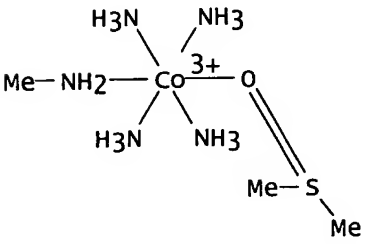
AN 116:50338 CA
TI Synthesis and characterization of trans-[Co(NH3)4(NH2CH3)L]3+ [L = (CH3)2SO or (CH3)2NCHO] complexes
AU Sienra, Beatriz; Massaferro, Adriana
CS Fac. Quim., Montevideo, Urug.
SO Polyhedron (1991), 10(17), 2075-8
CODEN: PLYHDE; ISSN: 0277-5387
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB trans-[Co(NH3)4(NH2Me)Me2SO]X3 (X = ClO4, Br) and trans-[Co(NH3)4(NH2Me)Me2NCHO](ClO4)3 are prepared by Ag+-induced solvolysis of trans-[Co(NH3)4(NH2Me)X]2+ (X = Cl or Br) complexes in DMSO or DMF. The complexes were characterized by electronic, IR and 1H NMR. DMSO and DMF are bonded through the oxygen atom. The trans-complexes obtained are not contaminated with the cis-isomers.
ST cobalt amine ammine DMF DMSO complex
IT 134066-28-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(dechlorination of, in DMSO)
IT 91321-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(dechlorination of, in DMSO or DMF)
IT 138521-44-5P 138521-45-6P 138521-47-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 64 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 138521-44-5 REGISTRY
ED Entered STN: 24 Jan 1992
CN Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-O]-, (OC-6-23)-, triperchlorate (9CI) (CA INDEX NAME)
MF C3 H23 Co N5 O S . 3 Cl O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

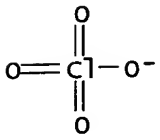
CM 1

CRN 138521-43-4
CMF C3 H23 Co N5 O S
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



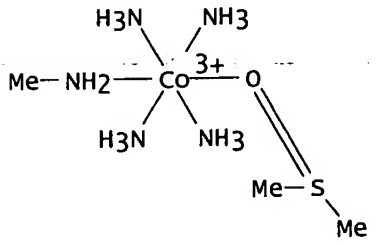
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 116:50338 CA
TI Synthesis and characterization of trans-[Co(NH3)4(NH2CH3)L]3+ [L = (CH3)2SO or (CH3)2NCHO] complexes
AU Sienra, Beatriz; Massaferro, Adriana
CS Fac. Quim., Montevideo, Urug.
SO Polyhedron (1991), 10(17), 2075-8
CODEN: PLYHDE; ISSN: 0277-5387
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)

AB trans-[Co(NH3)4(NH2Me)Me2SO]X3 (X = ClO4, Br) and trans-[Co(NH3)4(NH2Me)Me2NCHO](ClO4)3 are prepared by Ag+-induced solvolysis of trans-[Co(NH3)4(NH2Me)X]2+ (X = Cl or Br) complexes in DMSO or DMF. The complexes were characterized by electronic, IR and 1H NMR. DMSO and DMF are bonded through the oxygen atom. The trans-complexes obtained are not contaminated with the cis-isomers.
ST cobalt amine ammine DMF DMSO complex
IT 134066-28-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(dechlorination of, in DMSO)
IT 91321-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(dechlorination of, in DMSO or DMF)
IT 138521-44-5P 138521-45-6P 138521-47-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 65 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 138521-43-4 REGISTRY
ED Entered STN: 24 Jan 1992
CN Cobalt(3+), tetraammine(methanamine)[(sulfinyl-κO)bis[methane]]-, (OC-6-23)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-O]-, (OC-6-23)-
MF C3 H23 Co N5 O S
CI CCS, COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:142592 CA
TI Variable temperature and pressure study of the aquation reactions of cobalt(III) and chromium(III) penta- and tetra-amines
AU Benzo, Fabian; Bernhardt, Paul V.; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz
CS Facultad de Quimica, Catedra de Quimica Inorganica, Universidad de la Republica, Montevideo, 11800, Urug.
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (22), 3973-3979
CODEN: JCDTBI; ISSN: 0300-9246
PB Royal Society of Chemistry
DT Journal

LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB Preparation of a series of specific penta- and tetra-amine derivs. of CoIII and CrIII with a neutral leaving ligand has been carried out in order to accomplish a fine tuning of the associativeness/dissociativeness of their substitution reactions. Spontaneous aquation reactions of the neutral ligands have been studied at variable temperature and pressure. Although rate consts. and thermal activation parameters show an important degree of scatter, the values determined for the activation vols. of the substitution process illustrate the mechanistic fine tuning that may be achieved for these reactions. In all cases, in the absence of important steric constraints in the mol., electronic inductive effects seem to be the most important factor accounting for the dissociative shifts observed both for pentaamine i.e. ΔV.dbldag. = +4.0 or +14.0 cm3 mol-1 and +5.2 or +16.5 cm3 mol-1 for the aquation of cis- or trans-[Co(MeNH2)(NH3)4(DMF)]3+ and cis- or trans-[CoL15(DMF)]3+ resp., where L15 represents a pentaamine macrocyclic ligand, tetraamine systems i.e. ΔV.dbldag. = +4.1 or +8.4 cm3 mol-1 and -10.8 or -7.4 cm3 mol-1 for the aquation of cis-[Co(NH3)4Cl(DMAC)]2+ (DMAC = dimethylacetamide) or cis-[Co(en)2Cl(DMAC)]2+ and cis-[Cr(NH3)4Cl(DMF)]2+ or cis-[Cr(en)2Cl(DMF)]2+. From the results, clear evidence is obtained which indicates that, only when the situation is borderline Ia/Id, or the steric demands are increased dramatically, dissociative shifts are observed; in all other cases electronic inductive effects seem to be dominant for such a tuning of the substitution process.
ST cobalt amine complex aquation variable temp pressure; chromium amine complex aquation variable temp pressure
IT Activation enthalpy
Activation entropy
Activation volume
Aquation
Aquation kinetics
(variable temperature and pressure study of aquation reactions of cobalt(III) and chromium(III) penta- and tetra-amines)
IT 15696-63-6 15696-64-7 15696-65-8 19066-42-3 46240-37-3
59301-98-3 62728-45-4 62728-47-6 62728-54-5 62728-63-6
72382-37-7 72382-38-8 138521-43-4 138521-46-7 256652-23-0
256652-25-2 256652-28-5 256652-30-9 256652-32-1 256652-34-3
256652-35-4 256652-37-6 256652-39-8 256652-41-2 256652-43-4
256652-45-6 256652-47-8 256652-51-4 256656-89-0 256656-90-3
256656-91-4 256656-96-9
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(variable temperature and pressure study of aquation reactions of cobalt(III) and chromium(III) penta- and tetra-amines)
RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
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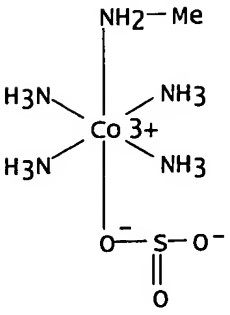
L9 ANSWER 66 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 134066-33-4 REGISTRY
ED Entered STN: 07 Jun 1991
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-O]-, (OC-6-23)-, nitrate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Sulfurous acid, cobalt complex
OTHER NAMES:
CN trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
MF C H17 Co N5 O3 S . N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

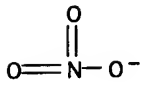
CRN 134066-32-3
CMF C H17 Co N5 O3 S

CCI CCS



CM 2

CRN 14797-55-8
CMF N O3



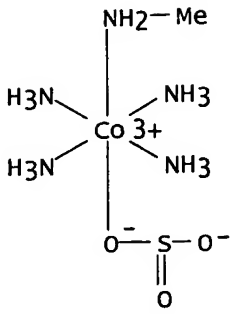
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 114:258445 CA
TI Synthesis, characterization and some reactions of trans-tetraamminebromo(methanamine)cobalt(2+) and trans-tetraammine(methanamine(nitratocobalt(2+) complexes
AU Sienra, B.; Massaferro, A.; Piriz Mac-Coll, C. R.
CS Univ. Republica, Montevideo, Urug.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1990), 590, 222-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB The preparation of trans-[Co(NH3)4(CH3NH2)Br]2+ (I) and trans-[Co(NH3)4(CH3NH2)(NO3)]2+ is described. The UV-visible spectra of the complexes indicate a decrease of the ligand field compared to the parent pentaammines. IR spectra match with the pattern of the corresponding pentaammines. The catalyzed (by Hg2+) aquation of I occurred with retention of the stereochem. configuration. The base hydrolysis (studied at 25°) products show trans to cis rearrangement for both complexes. 1H NMR spectroscopy is used for identification of the stereochem. configuration of the compds.
ST aquation cobalt ammine methanamine bromo complex; hydrolysis cobalt ammine methanamine complex isomerization; cobalt ammine methanamine complex
IT Isomerization
(in base hydrolysis of cobalt ammine methylamine complexes)
IT Aquation
(mercuric-catalyzed, of cobalt ammine methylamine complexes)
IT Hydrolysis

(base, of cobalt ammine methylamine complexes, isomerization in)
IT 134108-63-7P, cis-Tetraammineaqua(methylamine)cobalt(3+)
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in base hydrolysis of trans bromo complex with isomerization)
IT 134066-35-6P, trans-Tetraammineaqua(methylamine)cobalt(2+) perchlorate
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in catalyzed aquation of bromo complex)
IT 91321-36-7, trans-Tetraamminechloro(methylamine)cobalt(2+) perchlorate
RL: RCT (Reactant); RACT (Reactant or reagent)
(mercuric-catalyzed aquation and reaction of, with mercuric nitrate)
IT 134066-29-8P, trans-Tetraamminebromo(methylamine)cobalt(2+) dibromide
134066-31-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anion exchange of)
IT 134096-89-2P, trans-Tetraammine(methylamine)nitratocobalt(2+) perchlorate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and base hydrolysis of)
IT 134066-33-4P, trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of, in presence of nitric acid)
IT 134066-28-7P, trans-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mercuric-catalyzed aquation and base hydrolysis of)
IT 100788-48-5P, trans-Tetraammineaqua(methylamine)cobalt(3+) perchlorate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with bromide)
IT 134066-26-5P, trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrogen bromide)
IT 134108-62-6P, cis-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 88587-77-3, trans-Tetraamminehydroxysulfitocobalt
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylamine bromide)

L9 ANSWER 67 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 134066-32-3 REGISTRY
ED Entered STN: 07 Jun 1991
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-κO]-, (OC-6-23)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-O]-, (OC-6-23)-
CN Sulfurous acid, cobalt complex
MF C H17 Co N5 O3 S
CI CCS, COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 133:79995 CA
TI Inductive effect of methyl groups on acidopentaaminecobalt(III) complexes
AU Benzo, Fabian; Beyer, Lothar; Bozoglian, Fernando; Hallmeier, Karl-Heinz; Sienra, Beatriz
CS Universidad de la Republica, Catedra de Quimica Inorganica, Montevideo, Urug.
SO Polyhedron (2000), 19(8), 971-974
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB Electron spectroscopy for chemical anal. (ESCA) was performed for [Co(NH3)5Cl](Clo4)2, trans-[Co(NH3)4(NH2CH3)Cl]-(Clo4) 2, [Co(NH2CH3)5Cl](Clo4)2 and trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) complexes. Comparison of the results for the complexes [Co(NH3)5Cl](Clo4)2 and trans-[Co(NH3)4(NH2CH3)Cl](Clo4)2 shows clearly the electronic influence (+I effect) of the methylamine group on the cobalt and through this on the chlorine atom in trans position. Comparison of [Co(NH2CH3)5Cl](Clo4)2 with trans-[Co(NH3)4(NH2CH3)Cl](Clo4)2 shows that methylation of the four cis-NH3 ligands does not produce a proportional decrease in the binding energy of the cobalt atom, while the electron d. of the chloro ligand is not affected. For the complex trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) the +I effect is almost completely compensated by the presence of the sulfato group in trans position. Acid dissociation consts. are also reported for [Co(NH3)5(OH2)]3+ and trans-[Co(NH3)4(NH2CH3)(OH2)]3 + ions. The implications of these results for the mechanism of the acid and base hydrolysis reactions of acidopentaaminecobalt(III) complexes are discussed. The preparation of the trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) complex through the trans-[Co(NH3)4(NH2CH3)(SO3)]+ precursor is also described.
ST inductive effect methyl group acido amine cobalt complex
IT Hydrolysis
(acid, mechanism; inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT Dissociation constant
(acid; inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT Hydrolysis
(base, mechanism; inductive effect of Me groups on

acidopentaaminecobalt(III) complexes)
IT Inductive effect
Methyl group
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT 15156-18-0 15392-60-6 91321-36-7 279674-00-9
RL: PRP (Properties)
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
IT 14403-82-8 68250-09-9 134066-32-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
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(5) Benzo, F; to be published in Inorg React Mechanims
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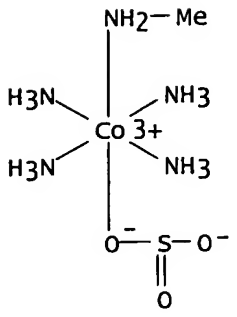
L9 ANSWER 68 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 134066-26-5 REGISTRY
ED Entered STN: 07 Jun 1991
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-O]-, bromide, (OC-6-23)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Sulfurous acid, cobalt complex
OTHER NAMES:
CN trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
MF C H17 Co N5 O3 S . Br
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
CRN (134066-32-3)



● Br^-

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

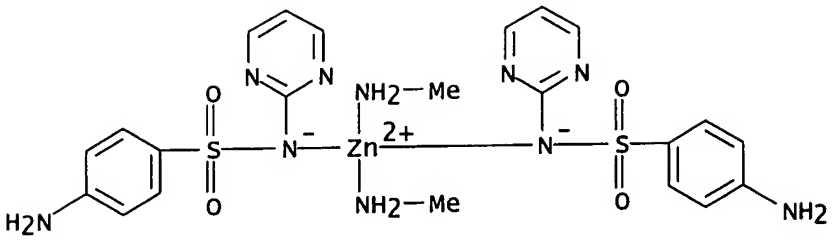
AN 114:258445 CA
TI Synthesis, characterization and some reactions of trans-tetraamminebromo(methanamine)cobalt(2+) and trans-tetraammine(methanamine(nitratocobalt(2+) complexes
AU Sienra, B.; Massaferro, A.; Piriz Mac-Coll, C. R.
CS Univ. Republica, Montevideo, Urug.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1990), 590, 222-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB The preparation of trans-[Co(NH3)4(CH3NH2)Br]2+ (I) and trans-[Co(NH3)4(CH3NH2)(NO3)]2+ is described. The UV-visible spectra of the complexes indicate a decrease of the ligand field compared to the parent pentaammines. IR spectra match with the pattern of the corresponding pentaammines. The catalyzed (by Hg2+) aquation of I occurred with retention of the stereochem. configuration. The base hydrolysis (studied at 25°) products show trans to cis rearrangement for both complexes. 1H NMR spectroscopy is used for identification of the stereochem. configuration of the compds.
ST aquation cobalt ammine methanamine bromo complex; hydrolysis cobalt ammine methanamine complex isomerization; cobalt ammine methanamine complex
IT Isomerization
(in base hydrolysis of cobalt ammine methylamine complexes)
IT Aquation
(mercuric-catalyzed, of cobalt ammine methylamine complexes)
IT Hydrolysis
(base, of cobalt ammine methylamine complexes, isomerization in)
IT 134108-63-7P, cis-Tetraammineaqua(methylamine)cobalt(3+)
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in base hydrolysis of trans bromo complex with isomerization)
IT 134066-35-6P, trans-Tetraammineaqua(methylamine)cobalt(2+) perchlorate
RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in catalyzed aquation of bromo complex)
IT 91321-36-7, trans-Tetraamminechloro(methylamine)cobalt(2+) perchlorate
RL: RCT (Reactant); RACT (Reactant or reagent)
(mercuric-catalyzed aquation and reaction of, with mercuric nitrate)
IT 134066-29-8P, trans-Tetraamminebromo(methylamine)cobalt(2+) dibromide
134066-31-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anion exchange of)
IT 134096-89-2P, trans-Tetraammine(methylamine)nitratocobalt(2+) perchlorate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and base hydrolysis of)
IT 134066-33-4P, trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and decomposition of, in presence of nitric acid)
IT 134066-28-7P, trans-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mercuric-catalyzed aquation and base hydrolysis of)
IT 100788-48-5P, trans-Tetraammineaqua(methylamine)cobalt(3+) perchlorate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with bromide)
IT 134066-26-5P, trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with hydrogen bromide)
IT 134108-62-6P, cis-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 88587-77-3, trans-Tetraamminehydroxysulfitocobalt
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylamine bromide)

L9 ANSWER 69 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 126830-36-2 REGISTRY
ED Entered STN: 27 Apr 1990
CN Zinc, bis(4-amino-N-2-pyrimidinylbenzenesulfonamidato)bis(methanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzenesulfonamide, 4-amino-N-2-pyrimidinyl-, zinc complex
MF C22 H28 N10 O4 S2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C4N2	NCNC3	6	C4N2	46.195.39	2



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

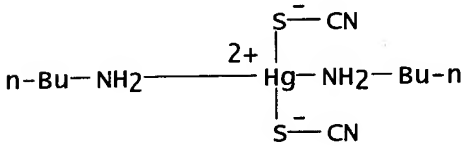
REFERENCE 1

AN 123:102111 CA
TI Zinc sulfadiazines: novel topical antimicrobial agents for burns
AU Lee, A. R.; Huang, W. H.
CS Sch. Pharmacy, National Defense Med. Cent., Taipei, Taiwan
SO Journal of Pharmacy and Pharmacology (1995), 47(6), 503-9
CODEN: JPPMAB; ISSN: 0022-3573
PB Royal Pharmaceutical Society of Great Britain
DT Journal
LA English
CC 1-5 (Pharmacology)
AB Two new zinc sulfadiazine (Zn(SD)2)-amine complexes, zinc sulfadiazine-methylamine (Zn(SD)2(CH3NH2)2) and zinc sulfadiazine-ethylenediamine (Zn(SD)2(C2H8N2)3.H2O), were prepared and compared with silver sulfadiazine (AgSD). The compds. were readily obtained by reaction of zinc nitrate hexahydrate with sulfadiazine or its methylamine and ethylenediamine salts. Structure was established by X-ray crystallog. and UV-visible, IR and NMR spectroscopy. The products were effective, in-vitro, against Gram-pos. and Gram-neg. bacteria as well as fungus. However, their activity is partially reversed by p-aminobenzoic acid. Further investigations in burned mice revealed that these compds. displayed a potential value in the prevention and treatment of wound healing, and diminution of mortality and weight loss. The toxicity of Zn(SD)2 derivs. was much lower than that of AgSD. The better aqueous solubility and skin permeability may explain the reason for their superiority over AgSD in the efficacy for topical therapy. Zn(SD)2(CH3NH2)2 was consistently more potent and was chosen for further development in clin. uses. The similarity in complexation between Sn(SD)2(CH3NH2)2 and AgSD may be significant to distinguish that from any other Zn(SD)2 derivative in bioactivity.
ST antimicrobial zinc sulfadiazine amine complex burn
IT Biocides
Burn
(zinc sulfadiazines and novel topical antimicrobial agents for burns)
IT 68-35-9, Sulfadiazine 547-32-0, Sulfadiazine sodium 10196-18-6, Zinc nitrate hexahydrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(zinc sulfadiazines and novel topical antimicrobial agents for burns)
IT 126830-35-1P 126830-36-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(zinc sulfadiazines and novel topical antimicrobial agents for burns)

REFERENCE 2

AN 112:209715 CA
TI A facile synthesis of zinc sulfadiazine derivatives
AU Lee, An Rong; Huang, Wen Hsin; Lai, Jin Shing; Chan, Shu Fei
CS Sch. Pharm., Natl. Def. Med. Cent., Taipei, Taiwan
SO Zhonghua Yaoxue Zazhi (1989), 41(4), 345-8
CODEN: CYHCEX; ISSN: 1016-1015
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 28
AB Treatment of sulfadiazine with Zn(NO3)2 in the presence of NH4OH, MeNH2, or H2NCH2CH2NH2 gave the corresponding title complexes, whose mol. structures were determined
ST zinc sulfadiazine amine complex; mol structure zinc sulfadiazine complex
IT Molecular structure
(of zinc-sulfadiazine-amine complexes)
IT 7779-88-6, Zinc nitrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with sulfadiazine and ammonia, methylamine, or ethylenediamine)
IT 68-35-9, Sulfadiazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with zinc nitrate and ammonia, methylamine, or ethylenediamine)
IT 88667-78-1P 126830-35-1P 126830-36-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

L9 ANSWER 70 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 110946-24-2 REGISTRY
ED Entered STN: 24 Oct 1987
CN Mercury, bis(1-butanamine-N)bis(thiocyanato-S)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, mercury complex
MF C10 H22 Hg N4 S2
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



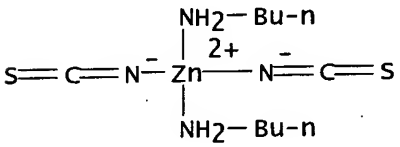
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 107:184014 CA
TI Study of the bond strength in complex compounds by proton NMR
AU Galitskaya, S. M.; Pavlenko, L. I.
CS USSR

SO Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
CODEN: VLPIAZ; ISSN: 0460-0436
DT Journal
LA Russian
CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 77
AB Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN, NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases in the order CN > NCS # NCSe.
ST bond energy complex NMR; zinc butylamine cyano complex bond energy; thiocyanato butylamine cadmium complex bond energy; selenocyanato butylamine cadmium complex bond energy; cadmium butylamine cyano complex bond energy; mercury butylamine cyano complex bond energy
IT Bond energy
(in Group IIB metal complexes, NMR in study of)
IT Nuclear magnetic resonance
(of Group IIB metal complexes)
IT 32491-81-9 32491-84-2 32491-88-6 38255-54-8 38271-02-2
110945-33-0 110946-24-2 110946-25-3 110987-94-5
RL: PRP (Properties)
(bond energy in, NMR in study of)

L9 ANSWER 71 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 110945-33-0 REGISTRY
ED Entered STN: 24 Oct 1987
CN Zinc, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, zinc complex
MF C10 H22 N4 S2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



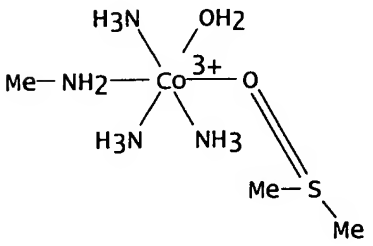
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 107:184014 CA
TI Study of the bond strength in complex compounds by proton NMR
AU Galitskaya, S. M.; Pavlenko, L. I.
CS USSR
SO Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
CODEN: VLPIAZ; ISSN: 0460-0436
DT Journal
LA Russian
CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 77
AB Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN, NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in

he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases in the order CN > NCS # NCSe.
ST bond energy complex NMR; zinc butylamine cyano complex bond energy; thiocyanato butylamine cadmium complex bond energy; selenocyanato butylamine cadmium complex bond energy; cadmium butylamine cyano complex bond energy; mercury butylamine cyano complex bond energy
IT Bond energy
(in Group IIB metal complexes, NMR in study of)
IT Nuclear magnetic resonance
(of Group IIB metal complexes)
IT 32491-81-9 32491-84-2 32491-88-6 38255-54-8 38271-02-2 110945-33-0 110946-24-2 110946-25-3 110987-94-5
RL: PRP (Properties)
(bond energy in, NMR in study of)

L9 ANSWER 72 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100838-97-9 REGISTRY
ED Entered STN: 15 Mar 1986
CN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-O]-, (OC-6-34)- (9CI) (CA INDEX NAME)
MF C3 H22 Co N4 O2 S
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)



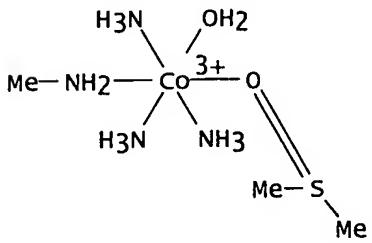
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 104:121904 CA
TI Formation and transformation of amminecarbonatocobalt(III) complexes
AU Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R.
CS Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB [CoCO3(NH3)5]Cl04.H2O, trans-[CoCO3(NH3)4(15NH3)]Cl04, and trans-[CoCO3(NH3)4(NH2Me)]Cl04 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. The products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific.
ST cobalt ammine carbonate prepn deammoniation; regiochem cobalt ammine

carbonato deammoniation
IT Substitution reaction
(internal, of cobalt ammine carbonato complexes, regiochem. of)
IT Regiochemistry
(of cobalt ammine carbonato complex internal substitution reactions of)
IT 100788-50-9P 100838-94-6P
RL: PREP (Preparation)
(formation by internal substitution reaction of tetramminecarbonato(methylamine)cobalt ion and aquation of)
IT 100788-51-0P 100838-95-7P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by aquation of carbonato complex)
IT 37549-01-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by internal substitution reaction of pentaamminecarbonatocobalt complex)
IT 100788-53-2P 100838-98-0P 100838-99-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from carbonato complex in acidified DMF)
IT 100788-52-1P 100838-96-8P 100838-97-9P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from carbonato complex in acidified DMSO)
IT 15244-74-3
RL: PROC (Process)
(ion exchange of, with perchlorate)
IT 91321-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(mercury ion-catalyzed aquation of)
IT 65774-48-3P 100788-47-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and internal substitution reaction of)
IT 100788-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with carbon dioxide)

L9 ANSWER 73 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100838-96-8 REGISTRY
ED Entered STN: 15 Mar 1986
CN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-O]-, (OC-6-43)- (9CI) (CA INDEX NAME)
MF C3 H22 Co N4 O2 S
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)



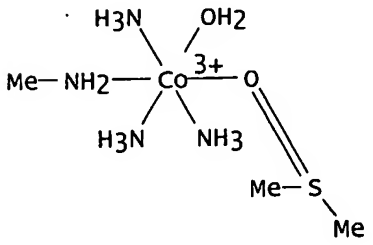
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 104:121904 CA
TI Formation and transformation of amminecarbonatocobalt(III) complexes
AU Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R.
CS Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB [CoCO3(NH3)5]ClO4.H2O, trans-[CoCO3(NH3)4(15NH3)]ClO4, and trans-[CoCO3(NH3)4(NH2Me)]ClO4 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. The products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific.
ST cobalt ammine carbonate prepn deammoniation; regiochem cobalt ammine carbonato deammoniation
IT Substitution reaction
(internal, of cobalt ammine carbonato complexes, regiochem. of)
IT Regiochemistry
(of cobalt ammine carbonato complex internal substitution reactions of)
IT 100788-50-9P 100838-94-6P
RL: PREP (Preparation)
(formation by internal substitution reaction of tetramminecarbonato(methylamine)cobalt ion and aquation of)
IT 100788-51-0P 100838-95-7P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by aquation of carbonato complex)
IT 37549-01-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by internal substitution reaction of pentaamminecarbonatocobalt complex)
IT 100788-53-2P 100838-98-0P 100838-99-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from carbonato complex in acidified DMF)
IT 100788-52-1P 100838-96-8P 100838-97-9P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from carbonato complex in acidified DMSO)
IT 15244-74-3
RL: PROC (Process)
(ion exchange of, with perchlorate)
IT 91321-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(mercury ion-catalyzed aquation of)
IT 65774-48-3P 100788-47-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and internal substitution reaction of)
IT 100788-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with carbon dioxide)

L9 ANSWER 74 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100788-52-1 REGISTRY
ED Entered STN: 08 Mar 1986

CN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-O]-, (OC-6-44)- (9CI) (CA INDEX NAME)
MF C3 H22 Co N4 O2 S
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 104:121904 CA
TI Formation and transformation of amminecarbonatocobalt(III) complexes
AU Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R.
CS Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB [CoCO3(NH3)5]ClO4.H2O, trans-[CoCO3(NH3)4(15NH3)]ClO4, and trans-[CoCO3(NH3)4(NH2Me)]ClO4 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. The products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific.
ST cobalt ammine carbonate prepn deammoniation; regiochem cobalt ammine carbonato deammoniation
IT Substitution reaction
(internal, of cobalt ammine carbonato complexes, regiochem. of)
IT Regiochemistry
(of cobalt ammine carbonato complex internal substitution reactions of)
IT 100788-50-9P 100838-94-6P
RL: PREP (Preparation)
(formation by internal substitution reaction of tetramminecarbonato(methylamine)cobalt ion and aquation of)
IT 100788-51-0P 100838-95-7P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by aquation of carbonato complex)
IT 37549-01-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by internal substitution reaction of pentaamminecarbonatocobalt complex)
IT 100788-53-2P 100838-98-0P 100838-99-1P
RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, from carbonato complex in acidified DMF)
IT 100788-52-1P 100838-96-8P 100838-97-9P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from carbonato complex in acidified DMSO)
IT 15244-74-3
RL: PROC (Process)
(ion exchange of, with perchlorate)
IT 91321-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(mercury ion-catalyzed aquation of)
IT 65774-48-3P 100788-47-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and internal substitution reaction of)
IT 100788-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with carbon dioxide)

L9 ANSWER 75 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100681-50-3 REGISTRY
ED Entered STN: 08 Mar 1986
CN Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-O]-, (OC-6-22)-, triperchlorate (9CI) (CA INDEX NAME)
MF C7 H31 Co N5 O S . 3 Cl O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

CRN 100681-48-9
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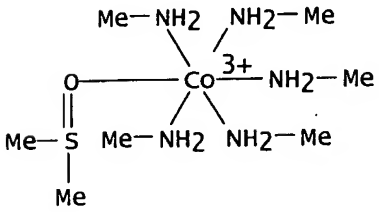
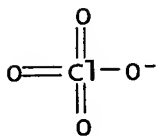
CCI CCS



CM 2

CRN 14797-73-0
CMF Cl O4



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

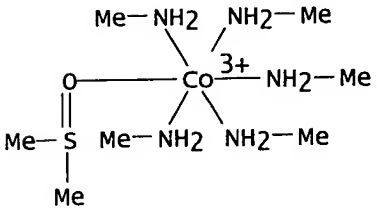
REFERENCE 1

AN 104:141030 CA
TI Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile
AU Curtis, Neville J.; Lawrance, Geoffrey A.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67
AB Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. ΔS.thermod. and ΔV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis(methylamine) complexes. These results parallel earlier observations of ΔS.thermod. and ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed.
ST cobalt methylamine neutral ligand complex; amine methyl cobalt neutral ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation; urea cobalt methylamine aquation
IT Aquation
Kinetics of aquation
(acid, of cobalt methylamine complexes with neutral ligands)
IT Steric effect
(in acid aquation of cobalt methylamine complexes with neutral ligands)
IT Hydrolysis
Kinetics of hydrolysis
(base, of cobalt acetonitrile methylamine complex)
IT 32424-84-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in acid aquation of cobalt methylamine neutral ligand complexes)
IT 100681-47-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of acid aquation and base hydrolysis of)
IT 100681-43-4P 100681-45-6P 100681-49-0P 100681-50-3P 100681-52-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and kinetics of acid aquation of)
IT 90065-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reactions of, with neutral ligands)

L9 ANSWER 76 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100681-49-0 REGISTRY
ED Entered STN: 08 Mar 1986
CN Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-O]-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Methanesulfonic acid, trifluoro-, ion(1-), (OC-6-22)-pentakis(methanamine)[sulfinylbis[methane]-O]cobalt(3+) (3:1)
MF C7 H31 Co N5 O S . 3 C F3 O3 S
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

CRN 100681-48-9
CMF C7 H31 Co N5 O S
CCI CCS



CM 2

CRN 37181-39-8
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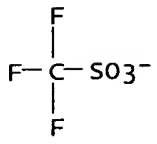


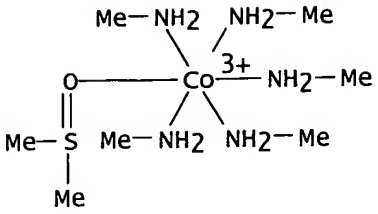
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 104:141030 CA
TI Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile
AU Curtis, Neville J.; Lawrance, Geoffrey A.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67
AB Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. ΔS.thermod. and ΔV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis(methylamine) complexes. These results parallel earlier observations of ΔS.thermod. and ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed.
ST cobalt methylamine neutral ligand complex; amine methyl cobalt neutral ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation; urea cobalt methylamine aquation
IT Aquation
Kinetics of aquation
(acid, of cobalt methylamine complexes with neutral ligands)
IT Steric effect
(in acid aquation of cobalt methylamine complexes with neutral ligands)
IT Hydrolysis
Kinetics of hydrolysis
(base, of cobalt acetonitrile methylamine complex)
IT 32424-84-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in acid aquation of cobalt methylamine neutral ligand complexes)
IT 100681-47-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of acid aquation and base hydrolysis of)
IT 100681-43-4P 100681-45-6P 100681-49-0P 100681-50-3P 100681-52-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and kinetics of acid aquation of)
IT 90065-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reactions of, with neutral ligands)

L9 ANSWER 77 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100681-48-9 REGISTRY
ED Entered STN: 08 Mar 1986
CN Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-O]-, (OC-6-22)-(9CI) (CA INDEX NAME)
MF C7 H31 Co N5 O S
CI CCS, COM
SR CA



L9 ANSWER 78 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100681-45-6 REGISTRY
ED Entered STN: 08 Mar 1986
CN Cobalt(3+), pentakis(methanamine)(trimethyl phosphate-O''')-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Methanesulfonic acid, trifluoro-, ion(1-), (OC-6-22)-pentakis(methanamine)(trimethyl phosphate-O''')cobalt(3+) (3:1)
CN Phosphoric acid, trimethyl ester, cobalt complex
MF C8 H34 Co N5 O4 P . 3 C F3 O3 S
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

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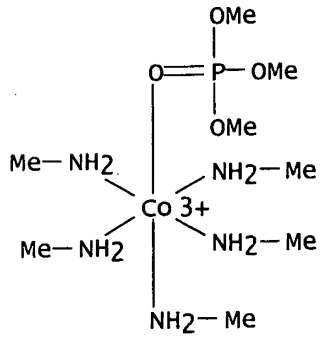
CRN 100681-44-5
CMF C8 H34 Co N5 O4 P
CCI CCS



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CRN 37181-39-8
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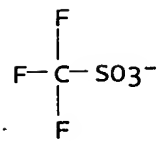
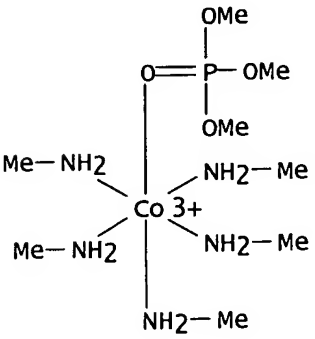


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 104:141030 CA
TI Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile
AU Curtis, Neville J.; Lawrance, Geoffrey A.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67
AB Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. ΔS.thermod. and ΔV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis(methylamine) complexes. These results parallel earlier observations of ΔS.thermod. and ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed.
ST cobalt methylamine neutral ligand complex; amine methyl cobalt neutral ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation; urea cobalt methylamine aquation
IT Aquation
Kinetics of aquation
(acid, of cobalt methylamine complexes with neutral ligands)
IT Steric effect
(in acid aquation of cobalt methylamine complexes with neutral ligands)
IT Hydrolysis
Kinetics of hydrolysis
(base, of cobalt acetonitrile methylamine complex)
IT 32424-84-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in acid aquation of cobalt methylamine neutral ligand complexes)
IT 100681-47-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of acid aquation and base hydrolysis of)
IT 100681-43-4P 100681-45-6P 100681-49-0P 100681-50-3P 100681-52-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and kinetics of acid aquation of)
IT 90065-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reactions of, with neutral ligands)

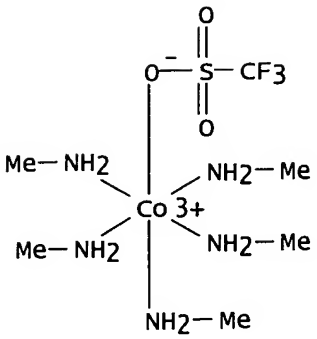
L9 ANSWER 79 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 100681-44-5 REGISTRY
ED Entered STN: 08 Mar 1986
CN Cobalt(3+), pentakis(methanamine)(trimethyl phosphate-O''')-, (OC-6-22)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phosphoric acid, trimethyl ester, cobalt complex
MF C8 H34 Co N5 O4 P
CI CCS, COM
SR CA



L9 ANSWER 80 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 90065-88-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Methanesulfonic acid, trifluoro-, ion(1-), (OC-6-22)-pentakis(methanamine)(trifluoromethanesulfonato-O)cobalt(2+) (2:1)
MF C6 H25 Co F3 N5 O3 S . 2 C F3 O3 S
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

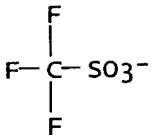
CM 1

CRN 84254-64-8
CMF C6 H25 Co F3 N5 O3 S
CCI CCS



CM 2

CRN 37181-39-8
CMF C F3 O3 S



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 105:107276 CA
TI Pentakis(methanamine)(trifluoromethanesulfonato-O) complexes of chromium(III), cobalt(III), and rhodium(III)
AU Lawrance, Geoffrey A.; Sargeson, Alan M.
CS Dep. Chem., Univ. Newcastle, 2308, Australia
SO Inorganic Syntheses (1986), 24, 279-82
CODEN: INSYA3; ISSN: 0073-8077
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB [M(NH2Me)5(OSO2CF3)](SO3CF3)2 (M = Co, Cr, Rh) were prepared from [M(NH2Me)5Cl]Cl2 and CF3SO3H.
ST safety transition metal methylamine trifluoromethanesulfonato
IT 90065-87-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from chromium chloro methylamine complex and trifluoromethane sulfonic acid)
IT 90065-88-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from cobalt chloro methylamine complex and trifluoromethanesulfonic acid)
IT 90065-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from rhodium chloro methylamine complex and trifluoromethanesulfonic acid)
IT 15351-84-5 15392-59-3 64459-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with trifluoromethanesulfonic acid)

REFERENCE 2

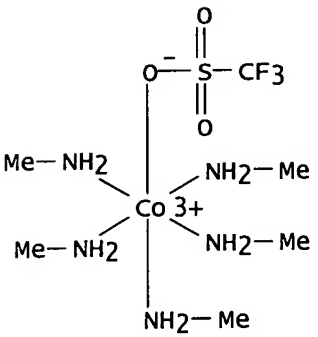
AN 104:141030 CA
TI Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile
AU Curtis, Neville J.; Lawrance, Geoffrey A.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67
AB Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. ΔS.thermod. and ΔV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis(methylamine) complexes. These results parallel earlier observations of ΔS.thermod. and ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed.
ST cobalt methylamine neutral ligand complex; amine methyl cobalt neutral ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation; urea cobalt methylamine aquation
IT Aquation
Kinetics of aquation
(acid, of cobalt methylamine complexes with neutral ligands)
IT Steric effect
(in acid aquation of cobalt methylamine complexes with neutral ligands)
IT Hydrolysis
Kinetics of hydrolysis
(base, of cobalt acetonitrile methylamine complex)
IT 32424-84-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in acid aquation of cobalt methylamine neutral ligand complexes)
IT 100681-47-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of acid aquation and base hydrolysis of)
IT 100681-43-4P 100681-45-6P 100681-49-0P 100681-50-3P 100681-52-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and kinetics of acid aquation of)
IT 90065-88-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reactions of, with neutral ligands)

REFERENCE 3

AN 101:121855 CA
TI Synthetically versatile (trifluoromethanesulfonato)metal amine complexes
AU Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan M.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia
SO Inorganic Chemistry (1984), 23(19), 2940-7
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67
AB Facile preparation routes to complexes of the labile unidentate coordinated -OSO2CF3 ion are reported for M(NH3)5(OSO2CF3)n+ (M = Rh, Ir, Cr, Ru, n = 2, M = Pt, n = 3), M(NH2Me)5(OSO2CF3)2+ (M = Co, Rh, Cr), cis-M(en)2(OSO2CF3)2+ (M = Rh, Ir, Cr, and trans-M(en)2Cl(OSO2CF3)+ (M = Rh, Ir). The utility of these synthetically versatile intermediates in the preparation of a variety of complexes containing neutral ligands is illustrated. Rate consts. for the aquation of the triflato complexes in 0.1M CF3SO3H at 25° span 3 orders of magnitude and for the pentaammine complexes show a reactivity order of Ru > Co .apprx. Cr .apprx. Rh » Ir > Pt. For the pentakis(methylamine) complexes, the aquation rate is greater for Co, slightly greater for Rh, and smaller for Cr in comparison to the corresponding pentaammine complexes. The aquations of M(en)2X(OSO2CF3)+ proceed largely without isomerization (<5%), and the triflato complexes are prepared stereospecifically by this route. For the cis-M(en)2(OSO2CF3)2+ ions, consecutive 1st-order aquation processes are observed with rate consts. k1 .apprx. 2k2.
ST transition metal amine trifluoromethanesulfonato; aquation kinetics amine trifluoromethanesulfonato complex; ammine transition metal trifluoromethanesulfonato; methylamine transition metal trifluoromethanesulfonato; ethylenediamine transition metal trifluoromethanesulfonato
IT Aquation
Kinetics of aquation
(of transition metal amine complexes with trifluoromethanesulfonate)
IT 75522-52-0
RL: PRP (Properties)
(kinetics of aquation of)
IT 84254-63-7P 90065-87-5P 90065-88-6P 90065-89-7P 90065-91-1P 90065-99-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of aquation of)
IT 14023-02-0P 15611-81-1P 29031-66-1P 32700-25-7P 87564-83-8P 90066-01-6P 90066-03-8P 90066-04-9P 90066-05-0P 90084-45-0P 90084-46-1P 90130-09-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 84254-57-9P 84254-59-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, aquation and reaction with ammonia)
IT 84254-61-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, aquation and reactions with acetonitrile and urea)
IT 90065-97-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reaction with ammonia and kinetics of aquation of)
IT 90065-95-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reaction with ethylenediamine and kinetics of aquation of)

IT 84278-98-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reaction with methanol and kinetics of aquation of)
IT 90065-93-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reactions with ammonia and ethylenediamine and kinetics of aquation of)
IT 13820-89-8 13820-95-6 14240-29-0 15351-84-5 15392-59-3
15444-46-9 15444-47-0 15444-62-9 15444-63-0 15742-38-8
16893-11-1 18532-87-1 64459-98-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with trifluoromethanesulfonic acid)

L9 ANSWER 81 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 84254-64-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-O)-, (OC-6-22)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Methanesulfonic acid, trifluoro-, cobalt complex
MF C6 H25 Co F3 N5 O3 S
CI CCS, COM
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties); RACT (Reactant or reagent)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 104:96513 CA
TI Hydrolysis of coordinated trifluoromethanesulfonate from cobalt(III), rhodium(III), iridium(III) and chromium(III) pentaamines
AU Curtis, Neville J.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan M.
CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
SO Inorganic Chemistry (1986), 25(4), 484-8
CODEN: INOCAJ; ISSN: 0020-1669
DT Journal
LA English
CC 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 78
AB Base hydrolysis and aquation of M(NH3)5(OSO2CF3)2+ (M = Co, Rh, Ir, Cr) and M(NH2CH3)5(OSO2CF3)2+ (M = Co, Rh, Cr) complexes at 25° and

ionic strength 1.0 M are reported. The N-methylation of the ammine ligand causes a marked enhancement of the rate of base hydrolysis reactions with kMe/kH of 2100 (Co), 150 (Rh), and 800 (Cr). Only minor enhancements occur for aquation with Co and Rh, while there is a minor rate diminution with Cr. Pos. activation entropies for base hydrolysis of M(NH3)5(OSO2CF3)2+ (M = Co, Ir) and competition expts. with azide ion in basic solution as well as the absence of the competing ion in the rate law allow a dissociative conjugate-base mechanism for all complexes. The variation in rate enhancement from ammine to methylamine compds. and the competition studies in base with azide ion chiefly reflect differences in steric interactions due to differing metal-ligand bond lengths rather than any mechanistic diversity. Variations in competition behavior for RhIII), Cr(III), and Co(III) appear to reflect relative lifetimes of the intermediate of reduced coordination number The variations in aquation are much smaller and do not allow any certainty in mechanistic assertions. Marked accelerations of rates for both acid and base hydrolyses (.apprx.103-106-fold) occur consistently for all trifluoromethanesulfonato complexes compared with those of halo of analogs.

ST hydrolysis kinetics rhodium 3 fluoromethanesulfonate; cobalt 3 ammine fluoromethanesulfonate hydrolysis; iridium 3 ammine fluoromethanesulfonate hydrolysis; chromium 3 ammine fluoromethanesulfonate hydrolysis

IT Transition metals, compounds
RL: USES (Uses)
(ammine or amine complexes containing trifluoromethanesulfonate, hydrolysis of)

IT Aquation
Hydrolysis
Kinetics of aquation
Kinetics of hydrolysis
(of transition metal ammine-trifluoromethanesulfonate complexes)

IT Ammines
RL: USES (Uses)
(transition metal, hydrolysis of trifluoromethanesulfonate ligand from)

IT 75522-49-5 84254-56-8 84254-58-0 84254-60-4 84254-64-8
84254-65-9 84254-66-0
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, kinetics of)

REFERENCE 2

AN 98:100163 CA

TI (Trifluoromethanesulfonato-O)pentaammine complexes: versatile synthetic intermediates

AU Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan M.

CS Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia

SO Inorganic Chemistry (1983), 22(5), 846-7
CODEN: INOCAJ; ISSN: 0020-1669

DT Journal

LA English

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 67

AB [M(NH3)5(OSO2CF3)](CF3SO3)n, where M = Cr(III), Rh(III), Ir(III), Ru(III), and Pt(IV), were prepared in essentially quant. yields from the reactions of [M(NH3)5Cl]Cln in CF3SO3H. The rate consts. for aquation of [M(NH3)5(OSO2CF3)](CF3SO3)n at 25° (0.1M CF3SO3H) indicate a reactivity order of Ru(III) > Rh(III) > Cr(III) > Pt(IV) > Ir(III). Aquation rate consts. for the [M(NH2Me)5(OSO2CF3)]2+ ions (M = Co(III), Rh(III), Cr(III)) were determined, and k(NH2Me)/k(NH3) ratios are 4.2, 1.7, and 0.051 for the Co(III), Rh(III), and Cr(III) complexes, resp.

ST ammine trifluoromethanesulfonato transition metal; chromium ammine

trifluoromethanesulfonato; rhodium ammine trifluoromethanesulfonato; iridium ammine trifluoromethanesulfonato; ruthenium ammine trifluoromethanesulfonato; platinum ammine trifluoromethanesulfonato; aquation kinetics transition metal trifluoromethanesulfonato

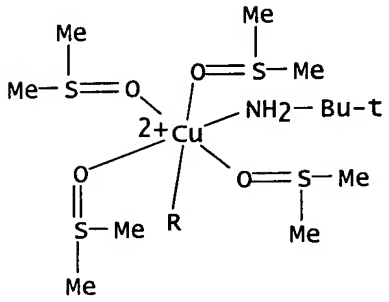
IT Kinetics of aquation
(of transition metal trifluoromethanesulfonato complexes)

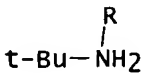
IT 84254-64-8 84254-65-9 84254-66-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(aquation of, kinetics of)

IT 84254-57-9P 84254-59-1P 84254-61-5P 84254-63-7P 84278-98-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of aquation of)

IT 13820-89-8 13820-95-6 15742-38-8 16893-11-1 18532-87-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with trifluoromethanesulfonic acid)

L9 ANSWER 82 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 73358-73-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper(2+), bis(2-methyl-2-propanamine)tetrakis[sulfinylbis[methane]-O]-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Propanamine, 2-methyl-, copper complex
MF C16 H46 Cu N2 O4 S4
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)





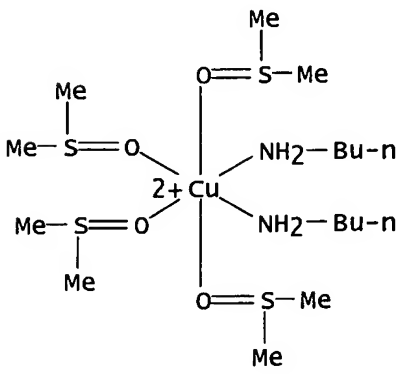
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 92:153821 CA
TI Complexing of copper(II) salts with pyridines and primary aliphatic amines in dimethyl sulfoxide
AU Dulova, V. I.; Brezhe, A. L.; Molchanova, N. R.; Artyukhova, E. P.
CS Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SO Koordinatsionnaya Khimiya (1980), 6(2), 248-51

CODEN: KOKHDC; ISSN: 0132-344X
DT Journal
LA Russian
CC 68-2 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
Section cross-reference(s): 69
AB Instability consts. were determined spectrophotometrically and heats of coordination were determined calorimetrically for 1:1 and 1:2 complexes by assuming equilibrium of the type Cu(DMSO)62+ + 2L .dblharw. Cu(DMSO)5L2+ + DMSO; Cu(DMSO)5L2+ + L .dblharw. Cu(DMSO)4L22+ + DMSO. The relative importance of bonding in these complexes is discussed.
ST copper amine complex stability DMSO; pyridine copper amine complex stability; thermodn coordination copper pyridine
IT Amines, compounds
RL: PRP (Properties)
(copper(II) complexes, in DMSO)
IT Entropy
(of coordination, of copper(II) with amines or pyridines in DMSO)
IT Formation constant and Stability constant
(of copper amine complexes, in DMSO)
IT Coordination
Heat of coordination
(of copper(II), with amines or pyridines in DMSO)
IT Substituent effect
(on stability, of copper amine and pyridine complexes in DMSO)
IT 73358-64-2P 73358-65-3P 73358-66-4P 73358-67-5P 73358-68-6P
73358-69-7P 73358-70-0P 73358-71-1P 73358-72-2P 73358-73-3P
73358-74-4P 73358-75-5P 73363-32-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in DMSO)

L9 ANSWER 83 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 73358-71-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper(2+), bis(1-butanamine)tetrakis[sulfinylbis[methane]-O]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex
MF C16 H46 Cu N2 O4 S4
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP (Preparation)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 92:153821 CA
TI Complexing of copper(II) salts with pyridines and primary aliphatic amines in dimethyl sulfoxide
AU Dulova, V. I.; Brezhe, A. L.; Molchanova, N. R.; Artyukhova, E. P.
CS Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SO Koordinatsionnaya Khimiya (1980), 6(2), 248-51
CODEN: KOKHDC; ISSN: 0132-344X
DT Journal
LA Russian
CC 68-2 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
Section cross-reference(s): 69
AB Instability consts. were determined spectrophotometrically and heats of coordination were determined calorimetrically for 1:1 and 1:2 complexes by assuming equilibrium of the type Cu(DMSO)62+ + 2L .dblharw. Cu(DMSO)5L2+ + DMSO; Cu(DMSO)5L2+ + L .dblharw. Cu(DMSO)4L22+ + DMSO. The relative importance of bonding in these complexes is discussed.
ST copper amine complex stability DMSO; pyridine copper amine complex stability; thermodn coordination copper pyridine
IT Amines, compounds
RL: PRP (Properties)
(copper(II) complexes, in DMSO)
IT Entropy
(of coordination, of copper(II) with amines or pyridines in DMSO)
IT Formation constant and Stability constant
(of copper amine complexes, in DMSO)
IT Coordination
Heat of coordination
(of copper(II), with amines or pyridines in DMSO)
IT Substituent effect
(on stability, of copper amine and pyridine complexes in DMSO)
IT 73358-64-2P 73358-65-3P 73358-66-4P 73358-67-5P 73358-68-6P
73358-69-7P 73358-70-0P 73358-71-1P 73358-72-2P 73358-73-3P
73358-74-4P 73358-75-5P 73363-32-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in DMSO)

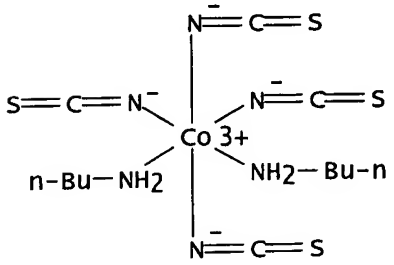
L9 ANSWER 84 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 67008-65-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-butanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, cobalt complex
CN 1-Propanamine, cobalt complex
CN 2-Pentanone, 4,4'-(1,2-ethanediyldinitrilo)bis-, cobalt complex
CN Cobaltate(1-), bis(1-butanamine)tetrakis(thiocyanato-N)-, (OC-6-11)-, (OC-6-22)-[[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)cobalt(1+) (9CI)
MF C18 H36 Co N4 O2 . C12 H22 Co N6 S4
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C2CoN2-C3CoNO-C3CoNO	CoNC2N-CoNC3O-CoNC3O	5-6-6	C8CoN2O2	1620.11.3	1 in CM 2

CM 1

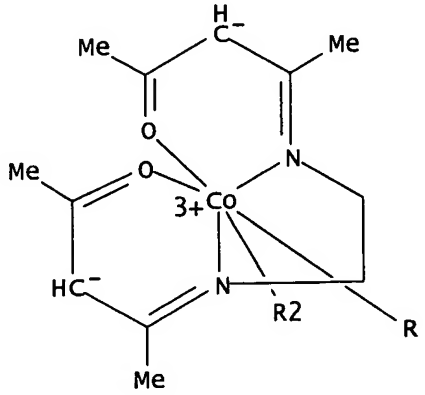
CRN 66915-23-9
CMF C12 H22 Co N6 S4
CCI CCS

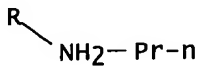


CM 2

CRN 30649-39-9
CMF C18 H36 Co N4 O2
CCI CCS

PAGE 1-A





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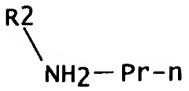


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 89:52589 CA
TI New tetrathiocyanatodiaminechromates with aliphatic monoamines
AU Ganescu, I.; Varhelyi, C.; Futo, F.; Brinzan, G.
CS Chem. Fak., Univ. Craiova, Craiova, Rom.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1978), 439, 282-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA German
CC 78-7 (Inorganic Chemicals and Reactions)
AB [Cr(NCS)4L2]- (L = PrNH2, BuNH2) were prepared by a substitution reaction of K3[Cr(NCS)6] with L in the molten state. Twenty complex salts of the type R.H[Cr(NCS)4L2] (L = amine) and 20 Co-amine complexes with [Co(NCS)4L2]- were isolated. The complexes were characterized by IR and UV spectra.
ST cobalt amine thiocyanato; propylamine cobalt thiocyanato; butylamine cobalt thiocyanato
IT 66915-18-2P 66915-20-6P 66915-21-7P 66915-24-0P 66915-25-1P
66915-26-2P 66915-27-3P 66915-28-4P 66915-29-5P 66915-30-8P
66915-32-0P 66915-33-1P 66915-34-2P 66915-35-3P 66915-36-4P
66915-37-5P 66915-38-6P 66915-39-7P 66915-41-1P 66915-42-2P
66915-43-3P 66915-44-4P 66915-45-5P 66915-46-6P 66915-47-7P
66964-00-9P 66969-90-2P 66969-92-4P 66969-93-5P 67008-64-4P
67008-65-5P 67008-66-6P 67008-67-7P 67008-68-8P 67008-69-9P
67008-70-2P 67008-71-3P 67146-74-1P 67146-75-2P 67146-76-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 85 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 67008-64-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-propanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, cobalt complex
CN 2-Pentanone, 4,4'-(1,2-ethanediyldinitrilo)bis-, cobalt complex
CN Cobaltate(1-), bis(1-propanamine)tetrakis(thiocyanato-N)-, (OC-6-11)-, (OC-6-22)-[[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)cobalt(1+) (9CI)
MF C18 H36 Co N4 O2 . C10 H18 Co N6 S4
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

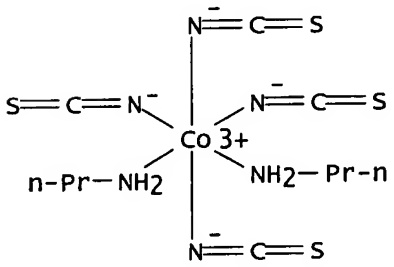
Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count

C2CoN2-C3CoNO-C3CoNO	CoNC2N-CoNC3O-CoNC3O	5-6-6	C8CoN2O2	1620.11.3	1 in CM 2

CM 1

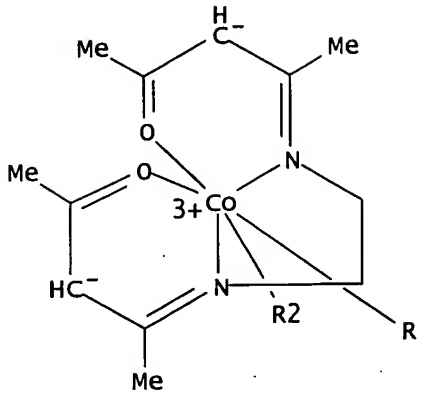
CRN 66915-22-8
CMF C10 H18 Co N6 S4
CCI CCS

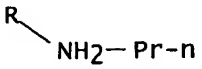


CM 2

CRN 30649-39-9
CMF C18 H36 Co N4 O2
CCI CCS

PAGE 1-A





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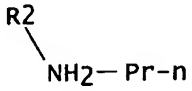
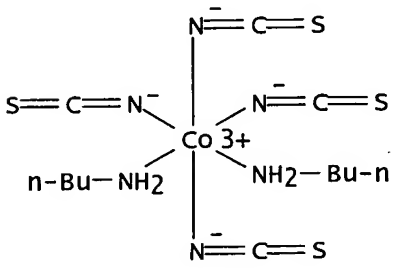


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

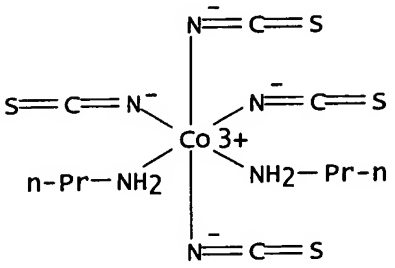
AN 89:52589 CA
TI New tetrathiocyanatodiaminechromates with aliphatic monoamines
AU Ganescu, I.; Varhelyi, C.; Futo, F.; Brinzan, G.
CS Chem. Fak., Univ. Craiova, Craiova, Rom.
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1978), 439, 282-8
CODEN: ZAACAB; ISSN: 0044-2313
DT Journal
LA German
CC 78-7 (Inorganic Chemicals and Reactions)
AB [Cr(NCS)4L2]- (L = PrNH2, BuNH2) were prepared by a substitution reaction of K3[Cr(NCS)6] with L in the molten state. Twenty complex salts of the type R.H[Cr(NCS)4L2] (L = amine) and 20 Co-amine complexes with [Co(NCS)4L2]- were isolated. The complexes were characterized by IR and UV spectra.
ST cobalt amine thiocyanato; propylamine cobalt thiocyanato; butylamine cobalt thiocyanato
IT 66915-18-2P 66915-20-6P 66915-21-7P 66915-24-0P 66915-25-1P
66915-26-2P 66915-27-3P 66915-28-4P 66915-29-5P 66915-30-8P
66915-32-0P 66915-33-1P 66915-34-2P 66915-35-3P 66915-36-4P
66915-37-5P 66915-38-6P 66915-39-7P 66915-41-1P 66915-42-2P
66915-43-3P 66915-44-4P 66915-45-5P 66915-46-6P 66915-47-7P
66964-00-9P 66969-90-2P 66969-92-4P 66969-93-5P 67008-64-4P
67008-65-5P 67008-66-6P 67008-67-7P 67008-68-8P 67008-69-9P
67008-70-2P 67008-71-3P 67146-74-1P 67146-75-2P 67146-76-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 86 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 66915-23-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobaltate(1-), bis(1-butanamine)tetrakis(thiocyanato-N)-, (OC-6-11)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, cobalt complex
MF C12 H22 Co N6 S4
CI CCS, COM

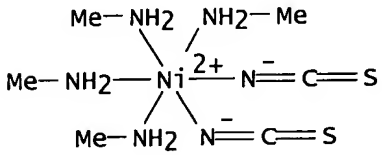


L9 ANSWER 87 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 66915-22-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobaltate(1-), bis(1-propanamine)tetrakis(thiocyanato-N)-, (OC-6-11)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

CN 1-Propanamine, cobalt complex
MF C10 H18 Co N6 S4
CI CCS, COM



L9 ANSWER 88 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61914-81-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(methanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA INDEX NAME)
MF C6 H20 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:83070 CA
TI Heterogeneous reactions of solid nickel(II) complexes. X. Study of stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-9 (Inorganic Chemicals and Reactions)
AB Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.

ST nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine thermal decompn
IT X-ray
(diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
IT 61896-84-2P 61896-86-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT 61896-80-8P 61896-82-0P
RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)
IT 55091-16-2 61876-10-6 61896-88-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

REFERENCE 2

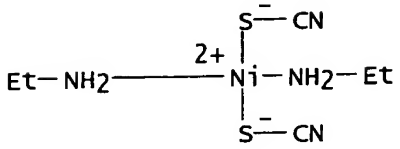
AN 86:83011 CA
TI Isomerism of nickel(II) complexes. VIII. Study of isomerism of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
AB Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2Me)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the monomer isomerizes to the green pseudooctahedral polymer. Steric effects in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic spectra.
ST nickel isothiocyanato amine complex isomerism; steric effect nickel isothiocyanato amine; thiocyanato nickel amine complex
IT Isomerism and Isomers
(of nickel isothiocyanato alkylamine complexes)
IT 55091-16-2P 61876-10-6P 61896-84-2P 61896-86-4P 61896-88-6P 61914-81-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 89 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-86-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, bis(ethanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethanamine, nickel complex, homopolymer
MF (C6 H14 N4 Ni S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

CRN 61896-85-3

CMF C6 H14 N4 Ni S2
CCI CCS



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:83070 CA
TI Heterogeneous reactions of solid nickel(II) complexes. X. Study of stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-9 (Inorganic Chemicals and Reactions)
AB Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.
ST nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine thermal decompn
IT X-ray
(diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
IT 61896-84-2P 61896-86-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT 61896-80-8P 61896-82-0P
RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)
IT 55091-16-2 61876-10-6 61896-88-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

REFERENCE 2

AN 86:83011 CA
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CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English

CC 78-7 (Inorganic Chemicals and Reactions)
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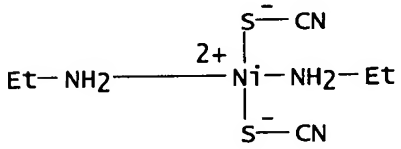
IT Isomerism and Isomers
(of nickel isothiocyanato alkylamine complexes)
IT 55091-16-2P 61876-10-6P 61896-84-2P 61896-86-4P 61896-88-6P 61914-81-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

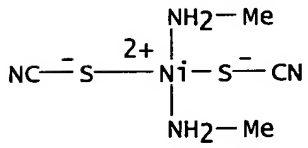
L9 ANSWER 90 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-85-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, bis(ethanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethanamine, nickel complex
MF C6 H14 N4 Ni S2
CI CCS, COM



L9 ANSWER 91 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-84-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)
MF (C4 H10 N4 Ni S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

CM 1

CRN 61896-83-1
CMF C4 H10 N4 Ni S2
CCI CCS



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:83070 CA
TI Heterogeneous reactions of solid nickel(II) complexes. X. Study of stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-9 (Inorganic Chemicals and Reactions)
AB Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.
ST nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine thermal decompn
IT X-ray
(diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
IT 61896-84-2P 61896-86-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT 61896-80-8P 61896-82-0P
RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)
IT 55091-16-2 61876-10-6 61896-88-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

REFERENCE 2

AN 86:83011 CA
TI Isomerism of nickel(II) complexes. VIII. Study of isomerism of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-7 (Inorganic Chemicals and Reactions)
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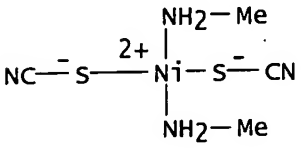
IT Isomerism and Isomers
(of nickel isothiocyanato alkylamine complexes)
IT 55091-16-2P 61876-10-6P 61896-84-2P 61896-86-4P 61896-88-6P
61914-81-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

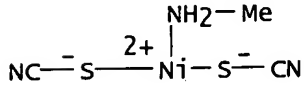
L9 ANSWER 92 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-83-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, bis(methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
MF C4 H10 N4 Ni S2
CI CCS, COM



L9 ANSWER 93 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-82-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, (methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
NAME)
MF (C3 H5 N3 Ni S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

CM 1

CRN 61896-81-9
CMF C3 H5 N3 Ni S2
CCI CCS



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 86:83070 CA
TI Heterogeneous reactions of solid nickel(II) complexes. X. Study of
stoichiometry of thermal decomposition of isothiocyanatonickel(II)
complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English

CC 78-9 (Inorganic Chemicals and Reactions)
AB Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.
ST nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine thermal decompn
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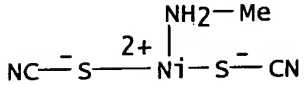
(diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
IT 61896-84-2P 61896-86-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT 61896-80-8P 61896-82-0P
RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)
IT 55091-16-2 61876-10-6 61896-88-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

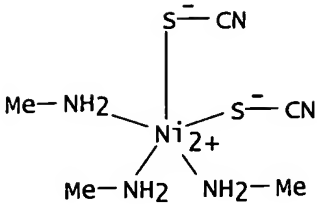
L9 ANSWER 94 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-81-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, (methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
MF C3 H5 N3 Ni S2
CI CCS, COM



L9 ANSWER 95 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-80-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tris(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)
MF (C5 H15 N5 Ni S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

CM 1

CRN 61896-79-5
CMF C5 H15 N5 Ni S2
CCI CCS

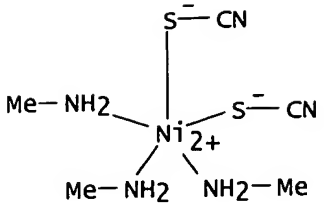


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

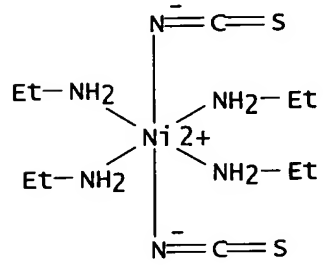
REFERENCE 1

AN 86:83070 CA
TI Heterogeneous reactions of solid nickel(II) complexes. X. Study of stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
AU Jona, E.; Vojtas, B.; Sramko, T.
CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-9 (Inorganic Chemicals and Reactions)
AB Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.
ST nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine thermal decompn
IT X-ray
(diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
IT 61896-84-2P 61896-86-4P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT 61896-80-8P 61896-82-0P
RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)
IT 55091-16-2 61876-10-6 61896-88-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

L9 ANSWER 96 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61896-79-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tris(methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
MF C5 H15 N5 Ni S2
CI CCS, COM



L9 ANSWER 97 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 61876-10-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(ethanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethanamine, nickel complex
MF C10 H28 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

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CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
CC 78-9 (Inorganic Chemicals and Reactions)
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ST nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine

thermal decompn
IT X-ray
(diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
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RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT 61896-80-8P 61896-82-0P
RL: PREP (Preparation)
(formation, x-ray diffraction and thermal decomposition of)
IT 55091-16-2 61876-10-6 61896-88-6 61914-81-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(thermal decomposition of)

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CS Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
SO Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
DT Journal
LA English
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(of nickel isothiocyanato alkylamine complexes)
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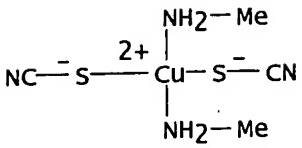
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 98 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 60865-94-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)
MF (C4 H10 Cu N4 S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Conference
RL.NP Roles from non-patents: PREP (Preparation)

CM 1

CRN 60865-93-2
CMF C4 H10 Cu N4 S2
CCI CCS

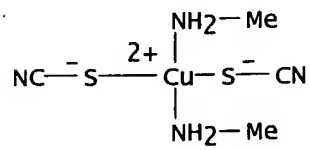


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 85:171027 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.
CS Kiev. Gos. Univ., Kiev, USSR
SO Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg. Khim., Novosibirsk, USSR.
CODEN: 34BFAN
DT Conference
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment.
ST copper amine selenocyanate thiocyanate; bipyridine copper selenocyanate thiocyanate; phenanthroline copper selenocyanate thiocyanate; ethylenediamine copper selenocyanate thiocyanate; butylamine copper selenocyanate thiocyanate; methylamine copper selenocyanate thiocyanate; propylamine copper selenocyanate thiocyanate
IT 19652-73-4P 22937-31-1P 60865-90-9P 60865-92-1P 60865-94-3P 60865-96-5P 60865-98-7P 60865-99-8P 60866-01-5P 60869-54-7P 60869-55-8P 60869-56-9P 60869-57-0P 60869-58-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 99 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 60865-93-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
MF C4 H10 Cu N4 S2
CI CCS, COM

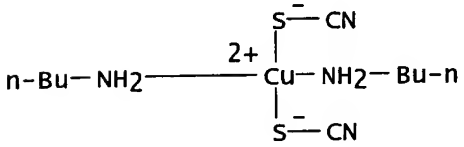


L9 ANSWER 100 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN

RN 60865-92-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-butanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex, homopolymer
MF (C10 H22 Cu N4 S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Conference
RL.NP Roles from non-patents: PREP (Preparation)

CM 1

CRN 60865-91-0
CMF C10 H22 Cu N4 S2
CCI CCS



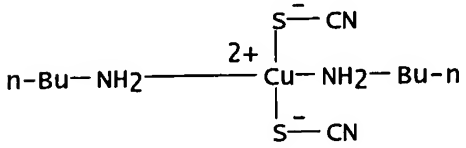
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 85:171027 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.
CS Kiev. Gos. Univ., Kiev, USSR
SO Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg. Khim., Novosibirsk, USSR.
CODEN: 34BFAN
DT Conference
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment.
ST copper amine selenocyanate thiocyanate; bipyridine copper selenocyanate thiocyanate; phenanthroline copper selenocyanate thiocyanate; ethylenediamine copper selenocyanate thiocyanate; butylamine copper selenocyanate thiocyanate; methylamine copper selenocyanate thiocyanate; propylamine copper selenocyanate thiocyanate
IT 19652-73-4P 22937-31-1P 60865-90-9P 60865-92-1P 60865-94-3P
60865-96-5P 60865-98-7P 60865-99-8P 60866-01-5P 60869-54-7P
60869-55-8P 60869-56-9P 60869-57-0P 60869-58-1P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

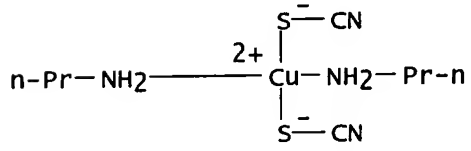
L9 ANSWER 101 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 60865-91-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-butanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex
MF C10 H22 Cu N4 S2
CI CCS, COM



L9 ANSWER 102 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 60865-90-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-propanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, copper complex, homopolymer
MF (C8 H18 Cu N4 S2)x
CI PMS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Conference
RL.NP Roles from non-patents: PREP (Preparation)

CM 1

CRN 60865-89-6
CMF C8 H18 Cu N4 S2
CCI CCS



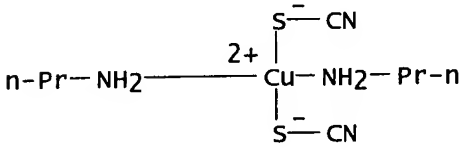
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 85:171027 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.
CS Kiev. Gos. Univ., Kiev, USSR
SO Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg. Khim., Novosibirsk, USSR.

CODEN: 34BFAN
DT Conference
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment.
ST copper amine selenocyanate thiocyanate; bipyridine copper selenocyanate thiocyanate; phenanthroline copper selenocyanate thiocyanate; ethylenediamine copper selenocyanate thiocyanate; butylamine copper selenocyanate thiocyanate; methylamine copper selenocyanate thiocyanate; propylamine copper selenocyanate thiocyanate
IT 19652-73-4P 22937-31-1P 60865-90-9P 60865-92-1P 60865-94-3P 60865-96-5P 60865-98-7P 60865-99-8P 60866-01-5P 60869-54-7P 60869-55-8P 60869-56-9P 60869-57-0P 60869-58-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 103 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 60865-89-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-propanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, copper complex
MF C8 H18 Cu N4 S2
CI CCS, COM



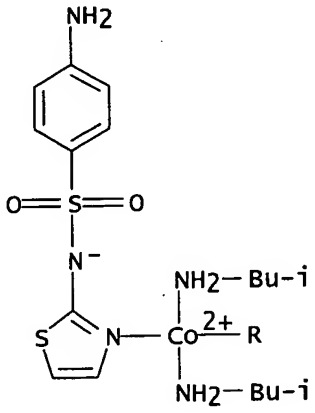
L9 ANSWER 104 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 59710-34-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt, bis(4-amino-N-2-thiazolylbenzenesulfonamidato-NN)bis(2-methyl-1-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, 2-methyl-, cobalt complex
CN Benzenesulfonamide, 4-amino-N-2-thiazolyl-, cobalt complex
MF C26 H38 Co N8 O4 S4
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence

EA	ES	SZ	RF	RID	Count
C3NS	NCSC2	5	C3NS	16.299.11	2
C6	C6	6	C6	46.150.18	2

PAGE 1-A



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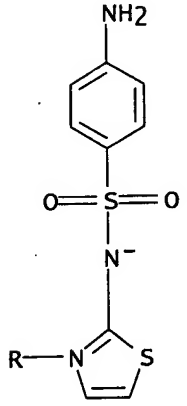


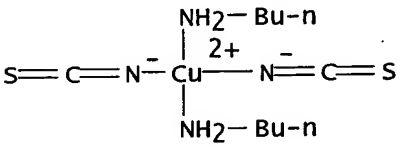
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 85:25322 CA
TI The cobaltous amine reaction. II. Cobalt complexes of barbiturates, methimazole, methylthiouracil, naphazoline, phenytoin, sulfathiazole and theophylline
AU Bult, A.
CS Lab. Pharm. Anal. Chem., State Univ. Groningen, Groningen, Neth.
SO Pharmaceutisch Weekblad (1976), 111(17), 385-93
CODEN: PHWEAW; ISSN: 0031-6911

DT Journal
LA English
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 64
AB The complexes of the composition CoX2(amine)2(X = anion of barbital, hexobarbital, methylphenobarbital, pentobarbital, phenobarbital, theophylline, and sulfathiazole; amine = isobutylamine, isopropylamine or NH3) are pseudo tetrahedral (Co(II) complexes. Co(II) coordinates with the barbiturates via N-I, with theophylline via N-7 or N-9, with sulfathiazole via the tertiary N atom of the thiazole ring. With X = anion of phenytoin the octahedral complex Co(II)X2(amine)4 is formed. This pink complex dissolves CHCl3 to a violet tetrahedral complex. With a large excess of amine the tetrahedral is converted to an octahedral. The donor atom in X is N-3. With X = naphazoline the (pseudo) tetrahedral Co(II) complexes CoX2(acetate)2 and [CoX4](ClO4)2 are prepared The pos. charge of Co2+ is compensated by acetate (coordinated) and ClO4- (uncoordinated resp. The donor atom in X is the tertiary Atom. With use of the ir spectra of previously described Co(II) complexes of methimazole a contribution to the interpretation of the ir spectrum of this drug is given. With X = anion of methylthiouracil some Co(III) complexes with the average composition CoX2(amine)n (n = .apprx.3) are prepared The available data
are insufficient for assigning the structure.
ST cobalt drug complex structure
IT Pharmaceuticals
(complexes with cobalt, preparation and mol. structure of)
IT Molecular structure
(of cobalt-pharmaceutical complexes)
IT 59448-18-9P 59448-19-0P 59448-20-3P 59653-28-0P 59680-97-6P
59681-00-4P 59710-33-7P 59710-34-8P 59710-35-9P 59710-37-1P
59710-39-3P 59710-40-6P 59710-41-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)

L9 ANSWER 105 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 57286-71-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex
MF C10 H22 Cu N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



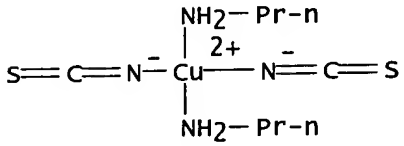
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 83:187668 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates

AU Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2, RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded. The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are N-bonded.
ST copper amine selenocyanate thiocyanate; bipyridine copper pseudohalogenide; phenanthroline copper pseudohalogenide
IT 19319-87-0P 22937-31-1P 25370-74-5P 57286-42-7P 57286-44-9P
57286-68-7P 57286-69-8P 57286-70-1P 57286-71-2P 57286-73-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 106 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 57286-70-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, copper complex
MF C8 H18 Cu N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

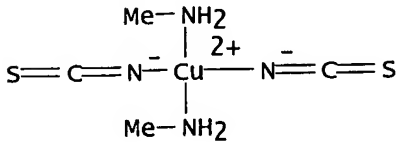
AN 83:187668 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2, RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded.

The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are N-bonded.

ST copper amine selenocyanate thiocyanate; bipyridine copper pseudohalogenide; phenanthroline copper pseudohalogenide

IT 19319-87-0P 22937-31-1P 25370-74-5P 57286-42-7P 57286-44-9P 57286-68-7P 57286-69-8P 57286-70-1P 57286-71-2P 57286-73-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 107 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 57286-68-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
MF C4 H10 Cu N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

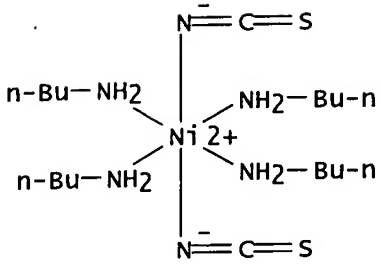
AN 125:24833 CA
TI Interaction of copper powder with nonaqueous solutions of methylammonium salts
AU Babich, O. A.; Kokozei, V. N.; Pavlenko, V. A.
CS Kiev. Gos. Univ., Kiev, Ukraine
SO Zhurnal Neorganicheskoi Khimii (1996), 41(1), 79-82
CODEN: ZNOKAQ; ISSN: 0044-457X
PB MAIK Nauka
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75
AB The interaction of Cu powder with MeCN, MeOH, DMSO, and DMF solns. of methylammonium bromide, iodide, or thiocyanate was studied. Products of the interaction were isolated and identified. The crystalline structure of [Cu(CH3NH2)4]I2 was detd (monoclinic, P21/n, a = 7.088(1), b = 8.872(1), c = 10.590(1) Å, β = 95.29(1)°, V = 663.04 Å3, Z = 2, ρc = 2.212 g/cm3, μ(CuKα) = 390.3 cm-1, F(000) = 414, T = 20°, 1043 reflections with I > 3σ(I), R = 0.061, Rw = 0.090).
ST copper reaction methylammonium salt nonaq solvent; crystal structure copper methylamine iodide
IT Crystal structure
Molecular structure
(of tetrakis(methylamine)copper(II) iodide)
IT 177604-59-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
IT 67-68-5DP, DMSO, copper thiocyanate methylamine complex 74-89-5DP,

Methylamine, copper DMSO thiocyanato complex 463-56-9DP, Thiocyanic acid , copper DMSO methylamine complex 7440-50-8DP, Copper, DMSO thiocyanato methylamine complex 57286-68-7P 177604-57-8P 177604-58-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation from Cu and methylammonium salts in nonaq. solns.)
IT 67-56-1, Methanol, uses 68-12-2, DMF, uses 75-05-8, Acetonitrile, uses
RL: NUU (Other use, unclassified); USES (Uses)
(reaction of Cu with nonaq. solns. of methylammonium salts)
IT 67-68-5, DMSO, reactions 6876-37-5, Methylammonium bromide 7440-50-8, Copper, reactions 14965-49-2, Methylammonium iodide 61540-63-4, Methylammonium thiocyanate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of Cu with nonaq. solns. of methylammonium salts)

REFERENCE 2

AN 83:187668 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2, RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded. The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are N-bonded.
ST copper amine selenocyanate thiocyanate; bipyridine copper pseudohalogenide; phenanthroline copper pseudohalogenide
IT 19319-87-0P 22937-31-1P 25370-74-5P 57286-42-7P 57286-44-9P 57286-68-7P 57286-69-8P 57286-70-1P 57286-71-2P 57286-73-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 108 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 54439-01-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, nickel complex
MF C18 H44 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

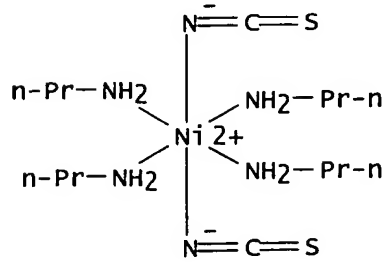


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 82:38050 CA
TI Nickel aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Amines in MeOH were added to MeOH-solns. containing KSCN or KSeCN and Ni(NO3)2.6-H2O to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined
ST selenocyanate nickel amine; nickel amine selenocyanate thiocyanate
IT 54438-96-9P 54438-97-0P 54438-98-1P 54438-99-2P 54439-00-8P
54439-01-9P 54439-03-1P 54495-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 109 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 54438-99-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
MF C14 H36 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

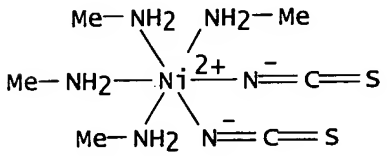


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 82:38050 CA
TI Nickel aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Amines in MeOH were added to MeOH solns. containing KSCN or KSeCN and Ni(NO3)2.6-H2O to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined
ST selenocyanate nickel amine; nickel amine selenocyanate thiocyanate
IT 54438-96-9P 54438-97-0P 54438-98-1P 54438-99-2P 54439-00-8P
54439-01-9P 54439-03-1P 54495-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 110 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 54438-97-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
MF C6 H20 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

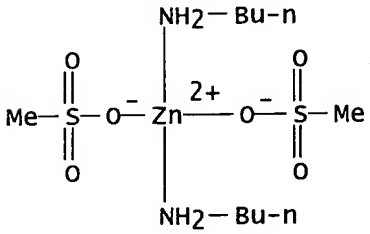
AN 82:38050 CA
TI Nickel aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB Amines in MeOH were added to MeOH solns. containing KSCN or KSeCN and Ni(NO3)2.6-H2O to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and

NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined

ST selenocyanate nickel amine; nickel amine selenocyanate thiocyanate

IT 54438-96-9P 54438-97-0P 54438-98-1P 54438-99-2P 54439-00-8P 54439-01-9P 54439-03-1P 54495-94-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 111 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 53396-13-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Zinc, bis(1-butanamine)bis(methanesulfonato-O)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, zinc complex
OTHER NAMES:
CN Bis(butylamine)bis(methanesulfonato)zinc
MF C10 H28 N2 O6 S2 Zn
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



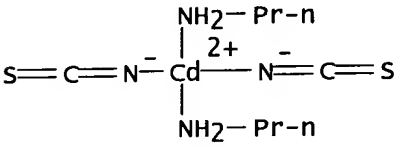
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 81:130234 CA
TI Chemistry of substituted sulfuric acids. VIII. Methanesulfonates of tin(II), tin(IV), and zinc(II)
AU Paul, Ram C.; Kapila, V. P.; Sharma, S. K.
CS Dep. Chem., Panjab Univ., Chandigarh, India
SO Indian Journal of Chemistry (1974), 12(6), 651-2
CODEN: IJOCAP; ISSN: 0019-5103
DT Journal
LA English
CC 78-5 (Inorganic Chemicals and Reactions)
AB $SnCl_2(MeSO_3)_2$, $Sn(MeSO_3)_2$, and $Zn(MeSO_3)_2$ were prepared by reacting the resp. metal chlorides with $MeSO_3H$. Their 1:2 adducts with pyridine and $BuNH_2$ were prepared and their conductances studied in $MeSO_3H$. The presence of phases $Cs_2M(MeSO_3)_4$ (M = Sn or Zn) was indicated by f.p. detns. of the $M(MeSO_3)_2$-$CsMeSO_3$ systems.
ST methanesulfonate tin zinc; pyridine tin zinc methanesulfonate; butylamine tin zinc methanesulfonate
IT 33684-80-9P 53396-08-0P 53396-09-1P 53396-10-4P 53396-11-5P 53396-12-6P 53396-13-7P 53408-93-8P 53408-94-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 112 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 38441-98-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cadmium, bis(1-propanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propanamine, cadmium complex
OTHER NAMES:
CN Cadmium, bis(isothiocyanato)bis(propylamine)-
MF C8 H18 Cd N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



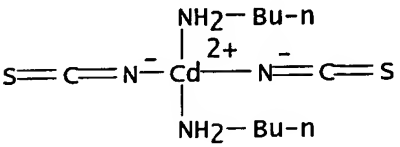
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:120272 CA
TI Cadmium aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Galitskaya, S. M.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
Section cross-reference(s): 78
AB The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu, do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to the Cd atom via the N atom.
ST IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
IT Molecular structure-property relationship
(ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate complexes)
IT Infrared spectra
(of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
IT 38255-49-1 38255-50-4 38255-51-5 38255-52-6 38255-53-7
38255-54-8 38271-02-2 38441-98-4
RL: PRP (Properties)
(ir spectrum of, structure in relation to)

L9 ANSWER 113 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 38255-54-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cadmium, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX

NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, cadmium complex
OTHER NAMES:
CN Cadmium, bis(butylamine)bis(isothiocyanato)-
MF C10 H22 Cd N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

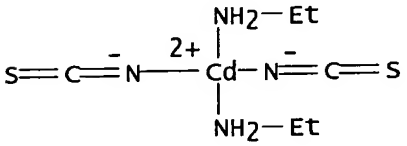
AN 107:184014 CA
TI Study of the bond strength in complex compounds by proton NMR
AU Galitskaya, S. M.; Pavlenko, L. I.
CS USSR
SO Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
CODEN: VLPIAZ; ISSN: 0460-0436
DT Journal
LA Russian
CC 65-5 (General Physical Chemistry)
Section cross-reference(s): 77
AB Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN, NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases in the order CN > NCS # NCSe.
ST bond energy complex NMR; zinc butylamine cyano complex bond energy; thiocyanato butylamine cadmium complex bond energy; selenocyanato butylamine cadmium complex bond energy; cadmium butylamine cyano complex bond energy; mercury butylamine cyano complex bond energy
IT Bond energy
(in Group IIB metal complexes, NMR in study of)
IT Nuclear magnetic resonance
(of Group IIB metal complexes)
IT 32491-81-9 32491-84-2 32491-88-6 38255-54-8 38271-02-2
110945-33-0 110946-24-2 110946-25-3 110987-94-5
RL: PRP (Properties)
(bond energy in, NMR in study of)

REFERENCE 2

AN 77:120272 CA
TI Cadmium aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Galitskaya, S. M.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian

CC 73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
Section cross-reference(s): 78
AB The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu, do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to the Cd atom via the N atom.
ST IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
IT Molecular structure-property relationship
(ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate complexes)
IT Infrared spectra
(of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
IT 38255-49-1 38255-50-4 38255-51-5 38255-52-6 38255-53-7
38255-54-8 38271-02-2 38441-98-4
RL: PRP (Properties)
(ir spectrum of, structure in relation to)

L9 ANSWER 114 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 38255-51-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cadmium, bis(ethanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ethanamine, cadmium complex
OTHER NAMES:
CN Cadmium, bis(ethylamine)bis(isothiocyanato)-
MF C6 H14 Cd N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)



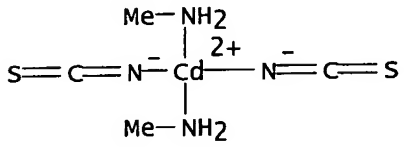
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:120272 CA
TI Cadmium aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Galitskaya, S. M.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
Section cross-reference(s): 78
AB The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu, do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to the Cd atom via the N atom.
ST IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR

IT Molecular structure-property relationship
(ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate complexes)
IT Infrared spectra
(of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
IT 38255-49-1 38255-50-4 38255-51-5 38255-52-6 38255-53-7
38255-54-8 38271-02-2 38441-98-4
RL: PRP (Properties)
(ir spectrum of, structure in relation to)

L9 ANSWER 115 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 38255-49-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cadmium, bis(methanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Cadmium, bis(isothiocyanato)bis(methylamine)-
MF C4 H10 Cd N4 S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)

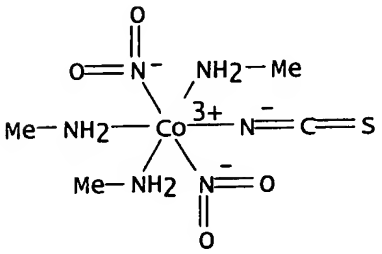


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:120272 CA
TI Cadmium aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Galitskaya, S. M.
CS Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SO Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
CODEN: UKZHAU; ISSN: 0041-6045
DT Journal
LA Russian
CC 73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
Section cross-reference(s): 78
AB The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu, do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to the Cd atom via the N atom.
ST IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
IT Molecular structure-property relationship
(ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate complexes)
IT Infrared spectra
(of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
IT 38255-49-1 38255-50-4 38255-51-5 38255-52-6 38255-53-7
38255-54-8 38271-02-2 38441-98-4
RL: PRP (Properties)
(ir spectrum of, structure in relation to)

L9 ANSWER 116 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 36741-31-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobalt, tris(methanamine)bis(nitrito-N)(thiocyanato-N)- (9CI) (CA INDEX NAME)
MF C4 H15 Co N6 O4 S
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



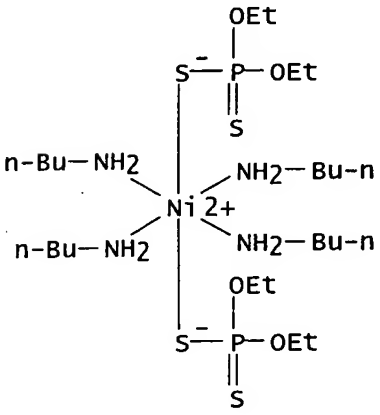
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 77:42560 CA
TI Nitro methylamine complexes of cobalt(III)
AU Ganiev, A. G.; Tukhtaev, Sh. Sh.; Ikramov, Kh. U.
CS Inst. Yad. Fiz., Kiev, USSR
SO Zhurnal Neorganicheskoi Khimii (1972), 17(5), 1384-7
CODEN: ZNOKAQ; ISSN: 0044-457X
DT Journal
LA Russian
CC 78-7 (Inorganic Chemicals and Reactions)
AB MeNH2 reacts with [Co(NO2)6]3- to give mixed complexes. K[Co(MeNH2)2(NO2)4], (CN3H5)H[Co(MeNH2)2(NO2)4], [Co(MeNH2)3(NO2)3], [Co(MeNH2)3(NO2)2(NCS)], [Co(MeNH2)2(NH3)(NO2)3], [Co(MeNH2)4(NO2)2][Co(NH3)2(NO2)4] were prepared The complexes of MeNH2 are less stable than the analogous NH3 complexes.
ST cobalt methylamine nitro complex; ammine cobalt
IT Ammines
RL: RCT (Reactant); RACT (Reactant or reagent)
(cobalt)
IT 19589-02-7P 36741-31-8P 36741-32-9P 36741-33-0P 36741-34-1P
36814-38-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L9 ANSWER 117 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 34406-41-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(butylamine)bis(dihydrogen phosphorodithioato)-, O,O,O,O-tetraethyl ester (8CI) (CA INDEX NAME)
MF C24 H64 N4 Ni O4 P2 S4
CI CCS
LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PRP (Properties)



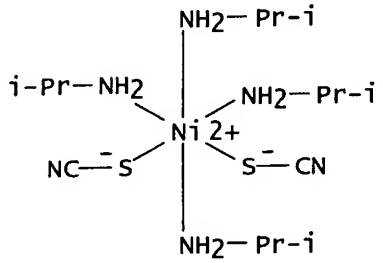
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 75:144420 CA
TI Stepwise adduct formation of bis(O,O'-diethyldithiophosphato)nickel(II) with primary and secondary amines
AU Ciullo, G.; Furlani, C.; Sestili, L.; Sgamellotti, A.
CS Inst. Gen. Inorg. Chem., Univ. Perugia, Perugia, Italy
SO Inorganica Chimica Acta (1971), 5(3), 489-92
CODEN: ICHAA3; ISSN: 0020-1693
DT Journal
LA English
CC 68 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
AB Bis(O,O'-diethyldithiophosphato)nickel(II) behaves in a qual. similar way with both primary and secondary amines in that 1:1 and 1:2 adducts are found. Data obtained for butylamine and diethylamine indicate that the difference in behavior towards primary and secondary amines is only quant., formation consts. being much smaller with the latter. Very high concn of primary amines leads also to the formation of complexes containing the chromophore (NiS2N4), presumably with monodentate dithiophosphate ligands.
ST nickel diethyldithiophosphate complex
IT Phosphorodithioic acid, O,O-diethyl ester, nickel complexes
RL: PRP (Properties); FORM (Formation, nonpreparative)
(formation consts. of)
IT 109-73-9D, Butylamine, nickel complexes 109-89-7D, Diethylamine, nickel complexes 29970-81-8 34406-41-2
RL: PRP (Properties); FORM (Formation, nonpreparative)
(formation consts. of)

L9 ANSWER 118 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 28067-98-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(isopropylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)
MF C14 H36 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS

DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)

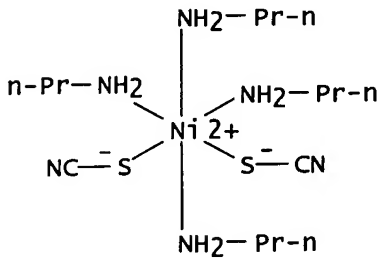


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 72:91917 CA
TI Separation of aromatic hydrocarbons using metal-organic complexes
AU Csikos, Rezso; Farkas, Peter
CS Hung.
SO Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10, 107-16
CODEN: MAFKAJ; ISSN: 0506-807X
DT Journal
LA Hungarian
CC 51 (Petroleum, Petroleum Derivatives, and Related Products)
AB Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their selectivity, and stability were examined
ST arom aliph hydrocarbons clathrate sepn; aliph arom hydrocarbons clathrate sepn; hydrocarbons arom aliph clathrate sepn
IT Nickel cyanide (Ni(CN)2), compound with ethylamine (1:1)
RL: USES (Uses)
(in benzene derivative separation from heptane)
IT 62-53-3D, Aniline, nickel complexes 75-04-7D, Ethylamine, nickel complexes 75-31-0D, Isopropylamine, nickel complexes 107-10-8D, Propylamine, nickel complexes 108-89-4D, 4-Picoline, nickel complexes 108-99-6D, 3-Picoline, nickel complexes 618-36-0D, Benzylamine, α-methyl-, nickel complexes 7004-58-2 14354-71-3 14875-85-5 26997-00-2 27256-97-9 27257-00-7, Ethylamine, compound with nickel cyanide (Ni(CN)2) (1:1) 27279-99-8 27910-87-8 27910-88-9 28067-98-3 28067-99-4 28631-77-8D, Pyridine, ethyl-, nickel complexes
RL: USES (Uses)
(in benzene derivative separation from heptane)
IT 142-82-5, uses and miscellaneous
RL: USES (Uses)
(separation of, from benzene derivs. by amine nickel complex)
IT 71-43-2P, preparation
RL: PREP (Preparation)
(separation of, from heptane by amine nickel complex)
IT 95-47-6 106-42-3, preparation 108-38-3, preparation
RL: PROC (Process)
(separation of, from heptane-xylene mixture by amine nickel complex)

L9 ANSWER 119 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 27910-88-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(propylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)
MF C14 H36 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)



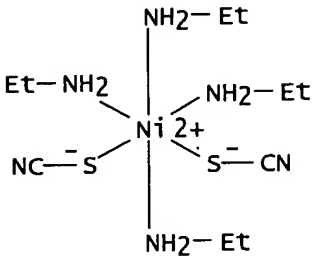
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 72:91917 CA
TI Separation of aromatic hydrocarbons using metal-organic complexes
AU Csikos, Rezso; Farkas, Peter
CS Hung.
SO Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10, 107-16
CODEN: MAFKAJ; ISSN: 0506-807X
DT Journal
LA Hungarian
CC 51 (Petroleum, Petroleum Derivatives, and Related Products)
AB Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their selectivity, and stability were examined
ST arom aliph hydrocarbons clathrate sepn; aliph arom hydrocarbons clathrate sepn; hydrocarbons arom aliph clathrate sepn
IT Nickel cyanide (Ni(CN)2), compound with ethylamine (1:1)
RL: USES (Uses)
(in benzene derivative separation from heptane)
IT 62-53-3D, Aniline, nickel complexes 75-04-7D, Ethylamine, nickel complexes 75-31-0D, Isopropylamine, nickel complexes 107-10-8D, Propylamine, nickel complexes 108-89-4D, 4-Picoline, nickel complexes 108-99-6D, 3-Picoline, nickel complexes 618-36-0D, Benzylamine, α-methyl-, nickel complexes 7004-58-2 14354-71-3 14875-85-5 26997-00-2 27256-97-9 27257-00-7, Ethylamine, compound with nickel cyanide (Ni(CN)2) (1:1) 27279-99-8 27910-87-8 27910-88-9 28067-98-3 28067-99-4 28631-77-8D, Pyridine, ethyl-, nickel complexes
RL: USES (Uses)
(in benzene derivative separation from heptane)
IT 142-82-5, uses and miscellaneous

RL: USES (Uses)
(separation of, from benzene derivs. by amine nickel complex)
IT 71-43-2P, preparation
RL: PREP (Preparation)
(separation of, from heptane by amine nickel complex)
IT 95-47-6 106-42-3, preparation 108-38-3, preparation
RL: PROC (Process)
(separation of, from heptane-xylene mixture by amine nickel complex)

L9 ANSWER 120 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 27910-87-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Nickel, tetrakis(ethylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)
MF C10 H28 N6 Ni S2
CI CCS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 72:91917 CA
TI Separation of aromatic hydrocarbons using metal-organic complexes
AU Csikos, Rezso; Farkas, Peter
CS Hung.
SO Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10, 107-16
CODEN: MAFKAJ; ISSN: 0506-807X
DT Journal
LA Hungarian
CC 51 (Petroleum, Petroleum Derivatives, and Related Products)
AB Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their selectivity, and stability were examined
ST arom aliph hydrocarbons clathrate sepn; aliph arom hydrocarbons clathrate sepn; hydrocarbons arom aliph clathrate sepn
IT Nickel cyanide (Ni(CN)2), compound with ethylamine (1:1)
RL: USES (Uses)
(in benzene derivative separation from heptane)
IT 62-53-3D, Aniline, nickel complexes 75-04-7D, Ethylamine, nickel complexes 75-31-0D, Isopropylamine, nickel complexes 107-10-8D, Propylamine, nickel complexes 108-89-4D, 4-Picoline, nickel complexes

108-99-6D, 3-Picoline, nickel complexes 618-36-0D, Benzylamine, α-methyl-, nickel complexes 7004-58-2 14354-71-3 14875-85-5 26997-00-2 27256-97-9 27257-00-7, Ethylamine, compound with nickel cyanide (Ni(CN)2) (1:1) 27279-99-8 27910-87-8 27910-88-9 28067-98-3 28067-99-4 28631-77-8D, Pyridine, ethyl-, nickel complexes
RL: USES (Uses)
(in benzene derivative separation from heptane)

IT 142-82-5, uses and miscellaneous
RL: USES (Uses)
(separation of, from benzene derivs. by amine nickel complex)

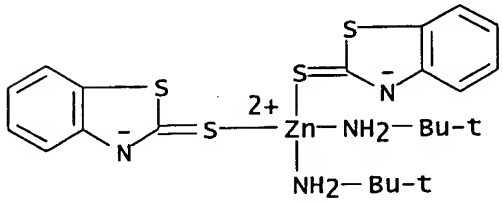
IT 71-43-2P, preparation
RL: PREP (Preparation)
(separation of, from heptane by amine nickel complex)

IT 95-47-6 106-42-3, preparation 108-38-3, preparation
RL: PROC (Process)
(separation of, from heptane-xylene mixture by amine nickel complex)

L9 ANSWER 121 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 15214-57-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Zinc, bis(2(3H)-benzothiazolethionato-κS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2(3H)-Benzothiazolethione, zinc complex
CN 2-Propanamine, 2-methyl-, zinc complex
CN Zinc, bis(2(3H)-benzothiazolethionato-S2)bis(2-methyl-2-propanamine)-, (T-4)-
CN Zinc, bis(2-benzothiazolethiolato)bis(tert-butylamine)- (7CI)
MF C22 H30 N4 S4 Zn
CI CCS
LC STN Files: CA, CAOLD, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3NS-C6	NCSC2-C6	5-6	C7NS	333.521.13	2



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475
PB American Chemical Society, Rubber Division
DT Journal
LA English
CC 39-10 (Synthetic Elastomers and Natural Rubber)
AB Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
ST sulfur vulcanization SBR quant structure property relationship
IT Molecular structure-property relationship
Sulfidation
Vulcanization
Vulcanization accelerators and agents
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT Styrene-butadiene rubber, processes
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-29-4 95-33-0 102-77-2 4979-32-2 7704-34-9, Sulfur, uses
10220-34-5 15214-44-5 15214-57-0 15670-77-6 26773-69-3
36930-73-1 37765-44-9 38335-52-3 38818-08-5 137376-19-3
156017-14-0 156477-90-6 157993-40-3 188036-96-6 252564-20-8
252564-21-9 252564-22-0 252564-23-1 252564-24-2 252564-25-3
252564-26-4 252564-27-5 252564-28-6 252564-29-7 252564-30-0
252564-31-1 252564-32-2 252564-33-3 252564-34-4 252564-35-5
252564-36-6 252564-37-7 252564-38-8 252564-83-3
RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 252564-18-4P
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 37143-54-7, 1-Methoxy-2-propylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
IT 9003-55-8

RL: PEP (Physical, engineering or chemical process); PROC (Process)
(styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
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REFERENCE 2

AN 64:33012 CA
TI Vulcanization accelerator-activator complexes. I. Amine complexes of zinc and cadmium benzothiazole-2-thiolate
AU Milligan, Brian
CS Nat. Rubber Producers' Res. Assoc., Welwyn Garden City, UK
SO J. Chem. Soc., Inorg., Phys., Theoret. (1966), (1), 34-5
DT Journal
LA English
CC 14 (Inorganic Chemicals and Reactions)
AB Eleven amine complexes of Zn benzothiazole-2-thiolate were prepared from the NH3 complex. Dissociation of the pyridine complex provides a convenient route to the thiolate, which is difficult to prepare by other methods.
IT Rubber
(vulcanization accelerator-activator complexes)
IT Rubber
(vulcanization accelerators for, 2-benzothiazolethiol complexes with Cd and Zn as)
IT Zinc, bis(2-benzothiazolethiolato)-, compound with ethylenediamine (1:3) tert-Butylamine, zinc complex with 2-benzothiazolethiol
RL: PREP (Preparation)
IT 108-91-8, Cyclohexylamine 110-89-4, Piperidine
(complexes of Cd and Zn with 2-benzothiazolethiol and)
IT 149-30-4, 2-Benzothiazolethiol
(complexes of Cd and Zn with amines and, rubber vulcanization accelerator-activator complexes)
IT 149-30-4, 2-Benzothiazolethiol
(complexes with Cd and Zn)
IT 97-39-2P, Guanidine, 1,3-di-o-tolyl-, zinc complex with 2-benzothiazolethiol 100-46-9P, Benzylamine, zinc complex with 2-benzothiazolethiol 102-06-7P, Guanidine, 1,3-diphenyl-, zinc complex with 2-benzothiazolethiol 107-15-3P, Ethylenediamine, compds. with bis(2-henzothtazolethiolato)zinc (3:1) 107-15-3P, Ethylenediamine, zinc complex with 2-benzothiazolethiol 110-86-1P, Pyridine, zinc complex with 2-benzothiazolethiol 110-91-8P, Morpholine, zinc complex with 2-benzothiazolethiol 141-43-5P, Ethanol, 2-amino-, zinc complex with 2-benzothiazolethiol 12194-64-8P, Zinc, bis(2-benzothiazolethiolato)bis(1,3-diphenylguanidine)- 12204-85-2P, Zinc, bis(2-benzothiazolethiolato)bis(1,3-di-o-tolylguanidine)- 14740-86-4P, Zinc, bis(2-benzothiazolethiolato)bis(pyridine)- 14807-72-8P, Cadmium, bis(2-benzothiazolethiolato)- 15214-44-5P, Zinc, bis(2-benzothiazolethiolato)bis(morpholine)- 15214-57-0P, Zinc, bis(2-benzothiazolethiolato)bis(tert-butylamine)- 15278-06-5P, Zinc, bis(2-benzothiazolethiolato)bis(2-aminoethanol)- 15612-28-9P, Cadmium, bis(2-benzothiazolethiolato)bis(piperidine)- 15627-29-9P, Zinc, bis(2-benzothiazolethiolato)bis(piperidine)- 15669-72-4P, Zinc, bis(2-benzothiazolethiolato)bis(benzylamine)- 15670-75-4P, Cadmium, bis(2-benzothiazolethiolato)bis(cyclohexylamine)- 15670-77-6P, Zinc,

bis(2-benzothiazolethiolato)bis(cyclohexylamine)- 15682-25-4P, Zinc,
bis(2-benzothiazolethiolato)(ethylenediamine)- 18907-31-8P, Zinc,
bis(2-benzothiazolethiolato)-
RL: PREP (Preparation)
(preparation of)

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FULL ESTIMATED COST	1.08	1373.41

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